Written test of Condensed Matter Physics - July 17th 2019

Profs. S. Caprara and A. Polimeni

$\hbar$=1.055x10^{-34} J·s, k_B=1.381x10^{-23} J/K.

Exercise 1. Potassium is a metal with the body-centered cubic (BCC) lattice structure with one atom basis. By performing a diffraction measurement using an x-ray beam with λ=0.116 nm, the first Bragg reflection compatible with the BCC structure is observed at the angle θ=8.85°. Evaluate:

a) the lattice parameter of the conventional cubic cell of potassium;

b) the Fermi energy (assuming a free-electron parabolic dispersion with the electron mass equal to that in vacuum).

Exercise 2. Consider a two-dimensional monoatomic crystal with square unit cell and lattice parameter equal to *a*=0.5 nm. Assume that the phonon dispersion can be accounted for by the Debye model, whereby all vibrational branches are replaced by the same linear dispersion relation $\omega = v \cdot |k|$, where *v*= 8000 m/s is the sound velocity. Determine:

a) the Debye temperature;

b) the expression and value of the specific heat at 5 K and at 5000 K.

Set $\int_0^\infty dx \cdot \frac{x^2}{e^x-1} = 2.4$

Exercise 1. Potassium is a metal with the body-centered cubic (BCC) lattice structure with one atom basis. By performing a diffraction measurement using an x-ray beam with λ=0.116 nm, the first Bragg reflection compatible with the BCC structure is observed at the angle θ=8.85°. Evaluate:

a) the lattice parameter of the conventional cubic cell of potassium;

b) the Fermi energy (assume the electron mass of electrons equal to that in vacuum).

a) $2dsin\theta = \lambda$, and for a BCC the first selection rule-compatible peak is for (hkl)=(110).

Thus, $a = d(1^2 + 1^2 + 0^2)^{1/2} = \frac{\lambda}{2sin\theta}\sqrt{2} = 0.533 \text{ nm}.$

b) $E_\text{F} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$, where n=2/(0.533 nm)^2=1.32×10^{28} m^{-3}. We obtain E_F=2.03 eV.

Exercise 2. Consider a two-dimensional monoatomic crystal with square unit cell and lattice parameter equal to a=0.5 nm. Assume that the phonon dispersion can be accounted for by the Debye model, whereby all vibrational branches are replaced by the same linear dispersion relation $\omega = v \cdot |k|$, where v= 8000 m/s is the sound velocity. Determine:

a) the Debye temperature;

b) the expression and value of the specific heat at 5 K and at 5000 K.

a) Like in three dimension, we replace the integral over the I Brillouin zone by an integral over a circle of radius k_D chosen to contain precisely the N allowed wave vectors, where N is the number of ions in the crystal. Since the area of k-space per allowed wave vector is $(2\pi)^2/S$ where S=a^2, this requires $(2\pi)^2 N/S$ to equal $\pi {k_\text{D}}^2$.

Therefore

$\pi k_\text{D}^2 = \frac{(2\pi)^2 N}{S} = \frac{(2\pi)^2}{a^2}$. Being $k_\text{D} = \frac{k_\text{B}\cdot\theta_\text{D}}{\hbar v}$, one finds $\theta_\text{D} = \frac{2v\hbar}{k_\text{B}}\frac{\sqrt{\pi}}{a} = 433 \text{ K}.$

b) $c_\text{V} = \frac{\partial}{\partial T}\sum_s \int_{IBZ}\frac{d^2\boldsymbol{k}}{(2\pi)^2}\cdot\frac{\hbar v_s k}{e^{\hbar v_s k/(k_\text{B}T)}}$ becomes $c_\text{V} = \frac{\partial}{\partial T} 2\int_0^{k_\text{D}}\frac{d^2\boldsymbol{k}}{(2\pi)^2}\cdot\frac{\hbar v k}{e^{\hbar v k/(k_\text{B}T)}}$. By making the change of variable $x = \frac{\hbar v}{k_\text{B}T}k$ and given $x_\text{D} = \frac{\hbar v}{k_\text{B}T}k_\text{D} = \frac{\theta_\text{D}}{T}$, one finds

$c_\text{V} = \frac{\partial}{\partial T}\frac{1}{\pi}\frac{(k_\text{B}T)^3}{(\hbar v)^2}\int_0^{\theta_\text{D}/T} dx\cdot\frac{x^2}{e^x - 1}$.

The 5 K and 5000 K represent the limits for which the following holds, respectively: $T \ll \theta_\text{D} (x \ll 1)$ and $T \gg \theta_\text{D} (x \gg 1)$.

- $T \ll \theta_\text{D} (x \ll 1)$.

$c_\text{V} = \frac{\partial}{\partial T}\frac{1}{\pi}\frac{(k_\text{B}T)^3}{(\hbar v)^2}\int_0^{\theta_\text{D}/T} dx\cdot\frac{x^2}{e^x-1} \rightarrow \frac{\partial}{\partial T}\frac{1}{\pi}\frac{(k_\text{B}T)^3}{(\hbar v)^2}\int_0^{\infty} dx\cdot\frac{x^2}{e^x-1} = \frac{2.4\cdot 3}{\pi}\frac{(k_\text{B})^3}{(\hbar v)^2}\cdot T^2$ given $\int_0^\infty dx\cdot\frac{x^2}{e^x-1} = 2.4.$

$c_\text{V} = \frac{2.4\cdot 3}{\pi}\frac{(k_\text{B})^3}{(\hbar v)^2}\cdot T^2 = \frac{12\cdot 2.4\cdot k_\text{B}}{a^2}\left(\frac{T}{\theta_\text{D}}\right)^2 = 2.12\cdot 10^{-7} \text{ J/(K}\cdot\text{m}^2).$

- $T \gg \theta_\text{D} (x \gg 1)$

In this case we have $\int_0^{\theta_\text{D}/T} dx\cdot\frac{x^2}{e^x-1} \approx \int_0^{\theta_\text{D}/T} dx\cdot\frac{x^2}{x}$ and consequently $c_\text{V} = \frac{\partial}{\partial T}\frac{1}{\pi}\frac{(k_\text{B}T)^3}{(\hbar v)^2}\frac{1}{2}\frac{(\theta_\text{D})^2}{(T)^2} = \frac{1}{2\pi}\frac{(k_\text{B})^3}{(\hbar v)^2}\theta_\text{D}^2 = \frac{2\cdot k_\text{B}}{a^2} = 1.11\cdot 10^{-4} \text{ J/(K}\cdot\text{m}^2).$