Written exam of Condensed Matter Physics - February 9th 2021
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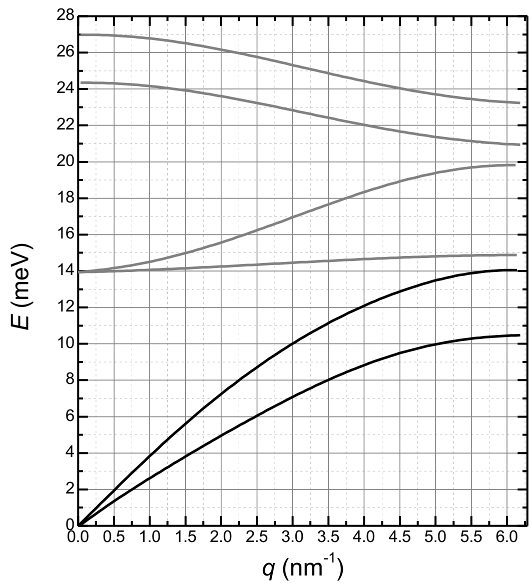
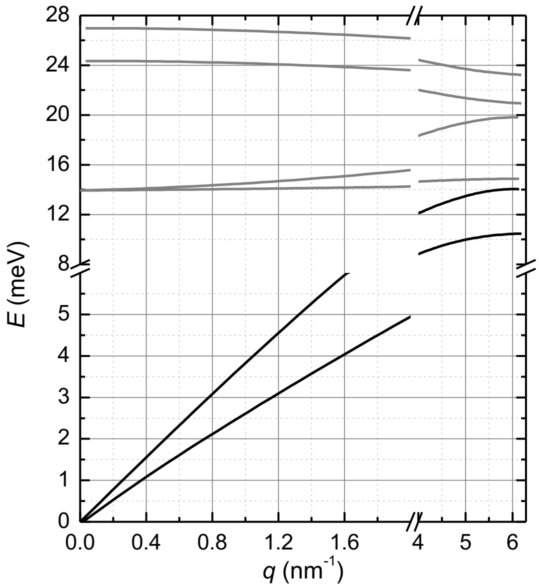
Exercise 1: Phonons [15 points]

A two-dimensional square lattice with lattice parameter a = 0.5 nm features the phonon dispersion curves shown in the figures below (the figure on the right is meant to highlight the low-q data). The atom motion is restricted in the lattice plane only (*i.e.*, no out-of-plane motion occurs).

1) Say if a basis is present and, if this is the case, the number of atoms it contains [2 points].
2) Estimate the values of the sound velocities [3 points].
3) Evaluate the specific heat value at 10 K justifying quantitatively the solution adopted [6 points].
4) Evaluate the Debye temperatures (note that the density that has to be considered is that corresponding to the Bravais lattice points and not to that of the atoms) and the specific heat at 1000 K [4 points].

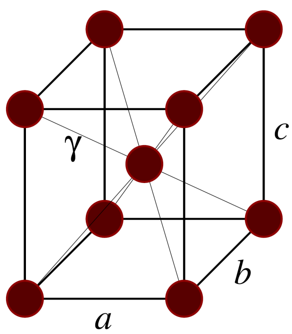
[Note that $\int_0^\infty \frac{x^2}{e^x-1} = 2.4$, k_B=1.381×10^{-23} J/K, $\hbar$=1.055×10^{-34} J·s].





Exercise 2: Tight binding [15 points]

Consider a body-centered orthorhombic crystal with sides of the conventional unit cell a = 0.28 nm, b = 0.30 nm, and c = 0.32 nm (see Figure on the right). Assume that the electron states can be described within the tight binding model with attractive potential $\Delta U < 0$ and the atoms contribute to the formation of the relevant electron band with s-type orbitals. The only transfer integral to be considered is for nearest-neighbors, γ = 0.25 eV [notice that in the given lattice $\frac{1}{2}\sqrt{a^2+b^2+c^2} < a, b, c$]. All other transfer integrals and all overlap integrals can be neglected. The atomic level is ε_s = 5.00 eV and β = 0.5 eV.



1) Determine the energy vs. quasi-momentum dispersion relation $E(\boldsymbol{k})$ [5 points].
2) Determine the position in quasi-momentum space and the energy of the maximum and minimum of the band [4 points].
3) Determine the expression and numerical values of the elements of the effective mass tensor at the Γ = (0,0,0) point of the Brillouin zone [6 points].

[Note that 1 eV corresponds to an energy of 1.602×10^{-19} J; the Planck constant is $\hbar$=1.055×10^{-34} J·s; the free electron mass is m_0 = 9.109×10^{-31} kg].

Solution Exercise 1

1) The observation of six phonon branches in a two-dimensional lattices implies the presence of a basis with 3 atoms.

2) The sound velocity can be estimated directly from the plot on the right hand side. We find: v_{s1}=5.61×10^3 m/s e v_{s2}=3.83×10^3 m/s.

3) The specific heat is given by

$c_v = \frac{\partial}{\partial T}\sum_{s=1,2}\int_{\mathrm{IBZ}}\frac{d^2\vec{q}}{(2\pi)^2}\frac{\hbar\omega_s(\vec{q})}{e^{\beta\hbar\omega_s(\vec{q})}-1}$.

For T=10 K, we have $k_B T$=0.863 meV. This implies that we are in the very low-T limit so that

$$c_v = \frac{\partial}{\partial T}\sum_{s=1,2}\int_0^\infty \frac{2\pi q dq}{(2\pi)^2}\frac{\hbar c_s q}{e^{\beta\hbar c_s q}-1}$$

$$= \sum_{s=1,2}\frac{{k_B}^3 3T^2}{2\pi(\hbar c_s)^2}\int_0^\infty dx\frac{x^2}{e^x-1} = 2.4\frac{3{k_B}^3T^2}{2\pi\hbar^2}\left(\frac{1}{v_{s1}^2}+\frac{1}{v_{s2}^2}\right)$$

$$= 2.71\times 10^{-6}\ \mathrm{J/(K\cdot m^2)}$$

4) For the Debye temperatures we have $\pi k_{\mathrm{D}}^2 = \frac{(2\pi)^2 N}{S} = \frac{(2\pi)^2}{a^2}$. Being $k_{\mathrm{D}} = \frac{k_{\mathrm{B}}\cdot\theta_{\mathrm{D}}}{\hbar v}$, one finds $\theta_{\mathrm{D1}} = \frac{2v_{s1}\hbar}{k_{\mathrm{B}}}\frac{\sqrt{\pi}}{a} = 303.8\ \mathrm{K}$ and $\theta_{\mathrm{D2}} = \frac{2v_{s2}\hbar}{k_{\mathrm{B}}}\frac{\sqrt{\pi}}{a} = 207.4\ \mathrm{K}$.

At T=1000 K, $c_{\mathrm{v}} = \frac{6\cdot k_{\mathrm{B}}}{a^2} = 3.32\cdot 10^{-4}\ \mathrm{J/(K\cdot m^2)}$.

Solution Exercise 2

1. Chosen the origin to coincide with the central atom in Fig. 2, the nearest neighbours are located at the 8 vertices of the conventional unit cell, corresponding to $\boldsymbol{R}=\left(\pm\frac{a}{2},\pm\frac{b}{2},\pm\frac{c}{2}\right)$. Then the dispersion law is

$$E(\boldsymbol{k})=\varepsilon_s-\beta-2\gamma\left[\cos\frac{k_xa+k_yb+k_zc}{2}+\cos\frac{k_xa+k_yb-k_zc}{2}+\cos\frac{k_xa-k_yb+k_zc}{2}+\cos\frac{k_xa-k_yb-k_zc}{2}\right]=\varepsilon_s-\beta-8\gamma\cos\frac{k_xa}{2}\cos\frac{k_yb}{2}\cos\frac{k_zc}{2}.$$

2. The derivatives of the energy dispersion relation are

$$\frac{\partial E(\boldsymbol{k})}{\partial k_x}=4\gamma a\sin\frac{k_xa}{2}\cos\frac{k_yb}{2}\cos\frac{k_zc}{2},$$

$$\frac{\partial E(\boldsymbol{k})}{\partial k_y}=4\gamma b\cos\frac{k_xa}{2}\sin\frac{k_yb}{2}\cos\frac{k_zc}{2},$$

$$\frac{\partial E(\boldsymbol{k})}{\partial k_z}=4\gamma c\cos\frac{k_xa}{2}\cos\frac{k_yb}{2}\sin\frac{k_zc}{2}.$$

The points where the cosines vanish cannot be maxima or minima, because these solutions give $E(\boldsymbol{k})=\varepsilon_s-\beta$. Then maxima and minima correspond to solutions where the sines vanish, $k_x=0,\frac{2\pi}{a}$, $k_y=0,\frac{2\pi}{b}$, $k_z=0,\frac{2\pi}{c}$. A minimum is found at the Γ point, where $E(\boldsymbol{k})=\varepsilon_s-\beta-8\gamma$. A maximum is found at $\left(\frac{2\pi}{a},0,0\right)$, $\left(0,\frac{2\pi}{b},0\right)$, $\left(0,0,\frac{2\pi}{c}\right)$, where $E(\boldsymbol{k})=\varepsilon_s-\beta+8\gamma$.

3. Expanding the dispersion around the Γ point, we find

$$E(\boldsymbol{k})\approx\varepsilon_s-\beta-8\gamma+\frac{2\gamma}{\hbar^2}\left(\frac{\hbar^2a^2k_x^2}{2}+\frac{\hbar^2b^2k_y^2}{2}+\frac{\hbar^2c^2k_z^2}{2}\right),$$

Whence it is evident that the mass tensor is diagonal and the only nonvanishing elements are

$$m_{xx}=\frac{\hbar^2}{2\gamma a^2}=1.771\times10^{-30}\text{ kg}=1.944\,m_0\,,$$

$$m_{yy}=\frac{\hbar^2}{2\gamma b^2}=1.543\times10^{-30}\text{ kg}=1.693\,m_0,$$

$$m_{zz}=\frac{\hbar^2}{2\gamma c^2}=1.356\times10^{-30}\text{ kg}=1.488\,m_0.$$