WRITTEN EXAM 22/04/2024 - Condensed Matter Physics - Profs. M. Grilli and A. Polimeni

EXERCISE 1

A one-dimensional crystal with lattice parameter a is formed by a diatomic basis containing an atom with mass m_1=1.795×10^{-26} kg and an atom with mass m_2=2.326×10^{-26} kg. The linear density of the lattice is λ=2.061×10^{-16} kg/m. The atoms in the lattice are coupled by first nearest neighbour interactions. The latter can be approximated by an elastic force with elastic constant C.

a) Knowing that the sound velocity in the lattice is v_s=1477.8 m/s, determine the optical phonon frequency at the centre of the first Brillouin zone.

b) Determine the Debye and the Einstein temperatures of the lattice.

c) Evaluate the specific heat of the lattice at T=1 K and T=900 K.

Note: $\int_0^\infty \mathrm{d}x \frac{x}{e^x-1} = \frac{\pi^2}{6}$ and $\int_0^\infty \mathrm{d}x \frac{x^2 e^x}{(e^x-1)^2} = \frac{\pi^2}{3}$ (only one of these should be used); k_B=1.381·10^{-23} J·K^{-1} $\hbar$=1.055·10^{-34} J·s.

EXERCISE 2

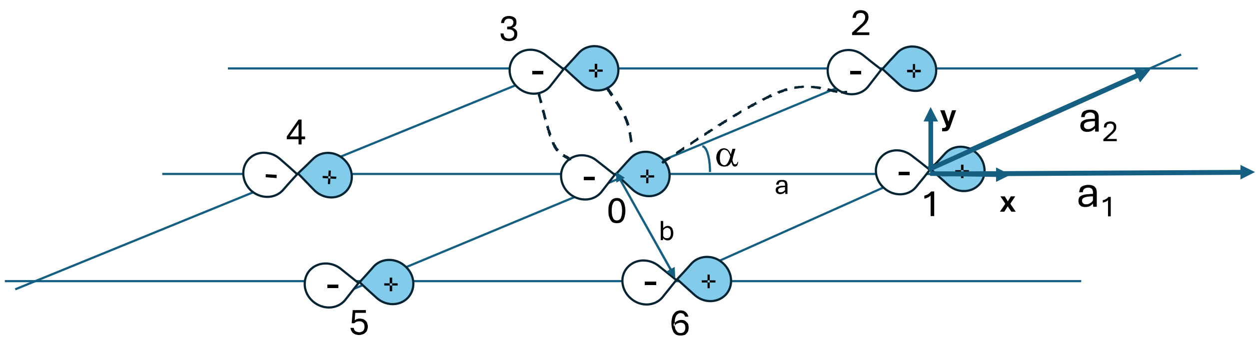
A two-dimensional lattice has a rhombic unit cell with lattice spacing a along x and a direction forming an angle $\alpha < 90^o$ with the x axis. On each site the ions have one p_x orbital (see figure). Notice that the 0-3 and 0-6 distance b is smaller than a. Using the tight-binding method indicate with $\gamma_{0,j}(\mathbf{R})$, $(j = 1-6)$ the nearest or next-nearest neighbour transfer integrals (hoppings) between the 0 and the j sites. The potential $\Delta U(\mathbf{r})$ is attractive.

i) Based on symmetry arguments, on the fact that the largest overlaps between the lobes of the orbitals are indicated by dashed lines, and by the fact that σ-like overlaps are larger than π-like ones, determine which transfer integrals $\gamma_{0,j}(\mathbf{R})$ are positive or negative, and assign the proper absolute values to the various $|\gamma_{0,j}(\mathbf{R})|$. In particular, for a given value of α, $t_1 = 1.1$ eV, $t_2 = 0.8$ eV, and $t_3 = 0.9$ eV;

ii) taking $E_0 \equiv E_{p_x} - \beta_{p_x} = 0$ and neglecting the overlap integrals $\alpha(\mathbf{R})$, write the general expression for the conduction band $E(\mathbf{k})$;

iii) consider the limit $\alpha \to \pi/2$. What kind of lattice do we have now? Considering that next-nearest neighbour hoppings are much smaller than nearest neighbour ones, order the hopping terms knowing that their absolute values are 1.1, 0.8, 0.01 eV. Calculate the Fermi level in the case of 1.99999 electrons per unit cell.

iv) For generic α write the unit vectors in the reciprocal lattice and their orientations with respect to $\mathbf{a}_{1,2}$.



Solution ex. 1

a) We know that for a one-dimensional lattice that the optical phonon frequency at the centre of the first Brillouin zone is $\omega_{\mathrm{opt}}(q=0)=\sqrt{2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}$.

The elastic constant C=4.5 kg/s^2 is found from the sound velocity $v_s=\sqrt{\frac{C/2}{(m_1+m_2)}}\,a$ with the lattice constant given by $a=\frac{(m_1+m_2)}{\lambda}$=0.200 nm. Hence, $\omega_{\mathrm{opt}}(q=0)=2.981\times10^{13}$ rad/s.

b) In the Debye model, we have $\omega_{\mathrm{D}}=q_{\mathrm{D}}v_{\mathrm{s}}=\frac{\pi}{a}v_{\mathrm{s}}=2.321\times10^{13}\,\frac{\mathrm{rad}}{\mathrm{s}}$ and the Debye temperature is $\Theta_{\mathrm{D}}=\frac{\hbar\omega_{\mathrm{D}}}{k_{\mathrm{B}}}$=177.3 K. In the Einstein model $\omega_{\mathrm{E}}=\omega_{\mathrm{opt}}(q=0)$ and the Einstein temperature is $\Theta_{\mathrm{E}}=\frac{\hbar\omega_{\mathrm{E}}}{k_{\mathrm{B}}}$=227.7 K.

c) We have two contributions to the internal energy density, one from the acoustic phonons and the other from the optical phonons:

$$u=\sum_{\mathrm{s=acoustic,optical}}\int_{-\pi/a}^{\pi/a}\frac{\mathrm{d}q}{2\pi}\frac{\hbar\omega_{\mathrm{s}}(q)}{e^{\beta\hbar\omega_{\mathrm{s}}(q)}-1}\approx\int_0^{q_{\mathrm{D}}}\frac{\mathrm{d}q}{\pi}\frac{\hbar v_{\mathrm{s}}q}{e^{\beta\hbar v_{\mathrm{s}}q}-1}+\frac{1}{a}\frac{\hbar\omega_{\mathrm{E}}}{e^{\beta\hbar\omega_{\mathrm{E}}}-1}.$$

For T=1 K, we have $k_{\mathrm{B}}T=0.086\ \mathrm{meV}\ll k_{\mathrm{B}}\Theta_{\mathrm{D}}(15.2\ \mathrm{meV}), k_{\mathrm{B}}\Theta_{\mathrm{E}}(19.6\ \mathrm{meV})$. The optical phonon contribution vanishes ($e^{\beta\hbar\omega_{\mathrm{E}}}\sim9.5\times10^{98}$) and the acoustic contribution can be expressed in terms of the frequency density of states $g(\omega)=\frac{1}{\pi v_{\mathrm{s}}}$

$u=\frac{1}{\pi v_{\mathrm{s}}}\int_0^{\omega_{\mathrm{D}}}\mathrm{d}\omega\,\frac{\hbar\omega}{e^{\beta\hbar\omega}-1}=\frac{k_{\mathrm{B}}^2T^2}{\hbar\pi v_{\mathrm{s}}}\int_0^{\Theta_{\mathrm{D}}/T=177}\mathrm{d}x\,\frac{x}{e^x-1}=\frac{k_{\mathrm{B}}^2T^2}{\hbar\pi v_{\mathrm{s}}}\frac{\pi^2}{6}$. Then, the specific heat is given by $c_{\mathrm{V}}=\frac{\partial u}{\partial T}=\frac{k_{\mathrm{B}}^2T}{\hbar v_{\mathrm{s}}}\frac{\pi}{3}=\frac{k_{\mathrm{B}}^2T}{\hbar\omega_{\mathrm{D}}}\frac{\pi^2}{3a}$=1.28×10^{-15} J/(K·m).

For T=900 K, $k_{\mathrm{B}}T=77\ \mathrm{meV}>k_{\mathrm{B}}\Theta_{\mathrm{D}}(15.2\ \mathrm{meV}), k_{\mathrm{B}}\Theta_{\mathrm{E}}(19.6\ \mathrm{meV})$ and the acoustic and optical phonon contributions equal, so that

$u\approx\frac{2k_{\mathrm{B}}T}{a}$ and $c_{\mathrm{V}}=\frac{2k_{\mathrm{B}}}{a}$=1.38×10^{-13} J/(K·m).

SOLUTION

i) The transfer integrals are given by:

$$\gamma_{0,1}=\gamma_{0,4}=-\int dr\psi^*(\mathbf{r})\Delta U(\mathbf{r})\psi(\mathbf{r}-\mathbf{R}_{1,4})=-t_1=-1.1<0$$

$$\gamma_{0,2}=\gamma_{0,5}=-\int dr\psi^*(\mathbf{r})\Delta U(\mathbf{r})\psi(\mathbf{r}-\mathbf{R}_{2,5})=-t_2=-0.8<0$$

$$\gamma_{0,3}=\gamma_{0,6}=-\int dr\psi^*(\mathbf{r})\Delta U(\mathbf{r})\psi(\mathbf{r}-\mathbf{R}_{3,6})=t_3=0.9>0$$

ii)

$$E(\mathbf{k})=2t_1\cos(ak_x)+2t_2\cos(ak_x\cos\alpha+ak_y\sin\alpha)-2t_3\cos(bk_x\sin\frac{\alpha}{2}-bk_y\cos\frac{\alpha}{2}),$$

where $b\equiv2a\sin\frac{\alpha}{2}$.

iii) In the limit $t_1>t_2\gg t_3$ and $\alpha\approx\pi/2$ the lattice becomes a simple cubic and the next-nearest neighbour hoppings $t_3=0.0001$ are assumed to be negligible. Then the maximum of the band occurs at $\mathbf{k}_M=(0,0)$ and $E_{MAX}=2t_1+2t_2=3.8$ eV. This is the Fermi level when the filling is approximately 2.

iv) Since $\mathbf{a}_1=a\mathbf{x}$ and $\mathbf{a}_2=a\cos\alpha\mathbf{x}+a\sin\alpha\mathbf{y}$, one finds that $|\mathbf{b}_{1,2}|=\frac{2\pi}{a\sin\alpha}$, with $\mathbf{b}_2$ // $\mathbf{y}$ and $\mathbf{b}_1$ rotated clockwise by $\pi/2-\alpha$ with respect to $\mathbf{x}$.