Written exam of Condensed Matter Physics - June 16th 2021
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Exercise 1: Phonons [15 points].

A metal with valence 3 features a simple cubic cell with a single-atom basis and an electron density $n_{\rm el} = 3.66 \times 10^{29}\,\mathrm{m}^{-3}$. The electrons can be treated as a gas of free particles. Concerning the metal ion vibrations, we have three acoustic branches (one longitudinal L and two transverse T) along the direction of the reciprocal lattice side:

$$\omega_{\rm T} = \omega_{\rm T}^0 \sin\left(\frac{qa}{2}\right), \qquad \omega_{\rm L} = \omega_{\rm L}^0 \sin\left(\frac{qa}{2}\right),$$

with $\omega_{\rm L}^0 = 4.8 \times 10^{12}$ rad/s. The Debye temperature of the transverse mode is $\Theta_{\rm T}^{\rm D} = 45.7\,\mathrm{K}$.

1. Determine the lattice constant a and the Debye wavevector $q_{\rm D}$ [**5 points**].

2. Determine the velocity of sound for longitudinal and transverse modes [**5 points**].

3. The low temperature specific heat at constant volume is given by $c_V(T) = A\,T + B\,T^3$.
Determine the value of A, B and of c_V at a temperature $T = 1\,\mathrm{K}$, knowing that the Fermi energy of the metal is $E_{\rm F} = 18.64\,\mathrm{eV}$ [**5 points**].

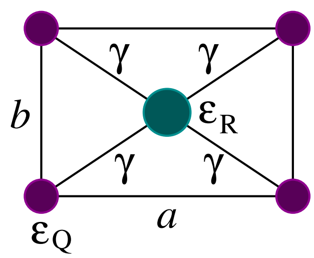

Fig. 1.

Exercise 2: Tight binding [15 points].

A two-dimensional rectangular crystal with lattice parameters $a = 0.4\,\mathrm{nm}$ and $b = 0.3\,\mathrm{nm}$ hosts the compound with chemical formula QR. The position of the Q atom within the primitive cell is identified by the basis vector $\boldsymbol{d}_{\rm Q} = (0,0)$, while the position of the R atom is identified by the basis vector $\boldsymbol{d}_{\rm R} = (\frac{a}{2}, \frac{b}{2})$. Assume that the electron states can be described within the tight binding model with attractive potential $\Delta U < 0$ and both atoms contribute to the formation of the relevant electron bands with s-type orbitals (see Fig. 1). The only transfer integral to be considered is $\gamma = 0.8\,\mathrm{eV}$, between Q atoms and nearest-neighboring R atoms (and viceversa). All other transfer integrals and all overlap integrals can be neglected. For simplicity, put to zero all the β integrals, and take the atomic levels $\varepsilon_{\rm Q} = 1.0\,\mathrm{eV}$ and $\varepsilon_{\rm R} = 3.0\,\mathrm{eV}$.

1. Determine the energy vs. quasi-momentum dispersion relations $E_\pm(\boldsymbol{k})$, where $+$ labels the conduction (upper) band and $-$ labels the valence (lower) band, and $\boldsymbol{k} = (k_x, k_y)$ [**5 points**].

2. Determine the position in quasi-momentum space and the energy of the maximum of the valence band and of the minimum of the conduction band. Determine the energy gap $E_{\rm g}$ between the valence band and the conduction band [**3 points**].

3. Determine the expression and numerical values of the elements of the effective mass tensors for the two bands at the $\Gamma = (0,0)$ point of the Brillouin zone [**7 points**].

[Note that $1\,\mathrm{eV}$ corresponds to an energy of 1.602×10^{-19} J; the Planck constant is $\hbar = 1.055\times10^{-34}$ J·s; the Boltzmann constant is $\kappa_B = 1.381 \times 10^{-23}$ J·K^{-1}; the free electron mass is $m_0 = 9.109 \times 10^{-31}$ kg].

Solution of the written exam
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Exercise 1.

1. The lattice constant is given by $a = n_{\rm at}^{-1/3} = 0.2016\,{\rm nm}$, where the atomic density is $n_{\rm at} = n_{\rm el}/3$. The Debye wavevector is $q_{\rm D} = (6\pi^2 n_{\rm at})^{1/3} = 1.933 \times 10^{10}\,{\rm m}^{-1}$.

2. The longitudinal sound velocity can be estimated as

$$v_{\rm L} = \lim_{q\to 0} \frac{{\rm d}\omega_{\rm L}}{{\rm d}q} = \frac{1}{2} a\omega_{\rm L}^0 = 483.8\,{\rm m/s}.$$

The transverse sound velocity is

$$v_{\rm T} = \frac{\kappa_B \Theta_{\rm T}^{\rm D}}{\hbar q_{\rm D}} = 309.5\,{\rm m/s}.$$

3. We know that the lattice contribution is $B\,T^3$, where

$$B = \frac{2\pi^2}{15}\frac{\kappa_B^4}{\hbar^3}\left(\frac{1}{v_{\rm L}^3} + \frac{2}{v_{\rm T}^3}\right) = 3.110 \times 10^3\,\frac{\rm J}{{\rm m}^3\cdot{\rm K}^4},$$

while the electronic contribution is $A\,T$, where

$$A = \frac{\pi^2}{2}\frac{\kappa_B^2}{E_{\rm F}} n_{\rm el} = 115.3\,\frac{\rm J}{{\rm m}^3\cdot{\rm K}^2}.$$

Therefore, the specific heat at $T = 1\,{\rm K}$ is $c_V = 3.225 \times 10^3\,{\rm J/(m^3\,K)}$.

Exercise 2.

1. The four vectors that locate the nearest-neighbor sites in the given lattice are $\boldsymbol{R} = (\pm\frac{a}{2}, \pm\frac{b}{2})$. Let

$$g_{\boldsymbol{k}} \equiv \gamma \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} = 4\gamma \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{bk_y}{2}\right).$$

Then, the coefficients $b_{\mathrm{Q}}, b_{\mathrm{R}}$ of the linear combination of atomic orbitals within the tight-binding method obey the set of linear equations

$$\begin{cases} [\varepsilon_{\mathrm{Q}} - E(\boldsymbol{k})]\, b_{\mathrm{Q}} - g_{\boldsymbol{k}} b_{\mathrm{R}} &= 0, \\ [\varepsilon_{\mathrm{R}} - E(\boldsymbol{k})]\, b_{\mathrm{R}} - g_{\boldsymbol{k}} b_{\mathrm{Q}} &= 0, \end{cases}$$

which has nontrivial solutions only if

$$E(\boldsymbol{k}) = \frac{\varepsilon_{\mathrm{Q}} + \varepsilon_{\mathrm{R}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + g_{\boldsymbol{k}}^2} \equiv E_{\pm}(\boldsymbol{k}).$$

2. The location of the maxima (minima) of the valence (conduction) band is given by the condition $g_{\boldsymbol{k}} = 0$, i.e., $k_x = \pm\frac{\pi}{a}$ or $k_y = \pm\frac{\pi}{b}$. These conditions correspond to the boundary of the first Brillouin zone. The values of the band energies are $E_+ = \varepsilon_{\mathrm{R}} = 3.0\,\mathrm{eV}$ and $E_- = \varepsilon_{\mathrm{Q}} = 1.0\,\mathrm{eV}$. The gap is $E_{\mathrm{g}} = \varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}} = 2.0\,\mathrm{eV}$.

3. Near the Γ point $g_{\boldsymbol{k}} \approx 4\gamma\left(1 - \frac{a^2k_x^2 + b^2k_y^2}{8}\right)$, and $g_{\boldsymbol{k}}^2 \approx 16\gamma^2\left(1 - \frac{a^2k_x^2 + b^2k_y^2}{4}\right)$. Then

$$E_{\pm} \approx \frac{\varepsilon_{\mathrm{R}} + \varepsilon_{\mathrm{Q}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2 - 4\gamma^2(a^2k_x^2 + b^2k_y^2)}$$

$$\approx \frac{\varepsilon_{\mathrm{R}} + \varepsilon_{\mathrm{Q}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2} \left[1 - \frac{2\gamma^2(a^2k_x^2 + b^2k_y^2)}{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2}\right].$$

Focusing on the $\boldsymbol{k}$-dependent part, we have

$$E_{\pm} \approx \ldots \mp \frac{2\gamma^2(a^2k_x^2 + b^2k_y^2)}{\sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2}} = \ldots \mp \left(\frac{\hbar^2k_x^2}{2m_{xx}^*} + \frac{\hbar^2k_y^2}{2m_{yy}^*}\right),$$

so the mass tensor at the Γ point is diagonal, with equal absolute value of the effective masses along the principal axes for both bands,

$$m_{xx}^* = \frac{\hbar^2\sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2}}{4\gamma^2a^2} = \sqrt{1 + \left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{8\gamma}\right)^2}\,\frac{\hbar^2}{\gamma a^2} = \frac{\sqrt{281}}{16}\frac{\hbar^2}{\gamma a^2} = 5.68 \times 10^{-31}\,\mathrm{kg} = 0.624\,m_0,$$

and

$$m_{yy}^* = \frac{\hbar^2\sqrt{\left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{2}\right)^2 + 16\gamma^2}}{4\gamma^2b^2} = \sqrt{1 + \left(\frac{\varepsilon_{\mathrm{R}} - \varepsilon_{\mathrm{Q}}}{8\gamma}\right)^2}\,\frac{\hbar^2}{\gamma b^2} = \frac{\sqrt{281}}{16}\frac{\hbar^2}{\gamma b^2} = 1.01 \times 10^{-30}\,\mathrm{kg} = 1.11\,m_0.$$