# Written exam of Condensed Matter Physics - April 20th 2021
## Profs. S. Caprara and A. Polimeni

**Exercise 1: X ray scattering and phonons [15 points].**

CuBr (cuprous bromide) crystallizes in the zincblende structure. The density of crystalline CuBr is $\rho_{\mathrm{CuBr}} = 4.71 \times 10^3$ kg·m$^{-3}$ and its molar mass is $\mu_{\mathrm{CuBr}} = 143.45 \times 10^{-3}$ kg·mol$^{-1}$.

1. Determine the side $a$ of the conventional cubic unit cell of CuBr [**4 points**].

2. The crystal structure of CuBr is investigated by means of X ray scattering within the Debye-Scherrer setup. The wavelength of the radiation is $\lambda = 0.1$ nm. Determine the scattering angles $\phi$ of the first 5 peaks that are compatible with the zincblende selection rules, and the corresponding indices $hkl$ of the cubic structure [**7 points**].

3. The velocity of sound of CuBr is $c_l = 3771$ m·s$^{-1}$ in the longitudinal acoustic phonon branch, and $c_{t1} = 1666$ m·s$^{-1}$ and $c_{t2} = 2020$ m·s$^{-1}$ in the two transversal acoustic phonon branches. Determine the average sound velocity $c_s$ (within the Debye approximation) and the Debye temperature $\Theta_D$ of the acoustic modes of CuBr [**4 points**].
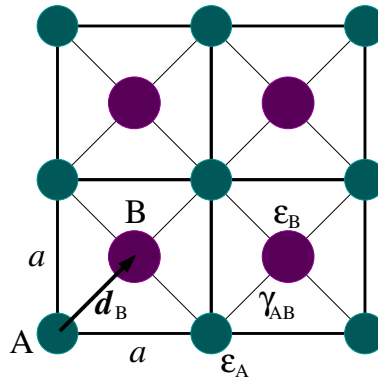


Fig. 1.

**Exercise 2: Tight binding [15 points].**

A two-dimensional square crystal with lattice constant $a = 0.45$ nm hosts the compound with chemical formula AB. The position of the A atom within the primitive cell is identified by the basis vector $\boldsymbol{d}_A = (0,0)$, while the position of the B atom is identified by the basis vector $\boldsymbol{d}_B = (\frac{a}{2}, \frac{a}{2})$. 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 $\gamma_{AB} = \gamma = 0.75$ eV, between A atoms and nearest-neighboring B atoms. All other transfer integrals and all overlap integrals can be neglected. For simplicity, put to zero all the $\beta$ integrals, and take the atomic levels $\varepsilon_A = 5.75$ eV and $\varepsilon_B = 5.00$ 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. [**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 eV corresponds to an energy of $1.602 \times 10^{-19}$ J; the Planck constant is $\hbar = 1.055 \times 10^{-34}$ J·s; the Avogadro number is $N_A = 6.022 \times 10^{23}$ mol$^{-1}$; 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].

**Exercise 1**.

1. The molar density of CuBr is

$$\rho_{\text{mol}} = \frac{\rho_{\text{CuBr}}}{\mu_{\text{CuBr}}} = 3.282 \times 10^4 \, \text{mol} \cdot \text{m}^{-3}.$$

Then, since in a conventional unit cell of the zincblende structure there are 4 CuBr molecules, the lattice constant of the conventional cubic unit cell of CuBr is $a = [4/(N_A \, \rho_{\text{mol}})]^{1/3} = 0.5871 \, \text{nm}$.

2. The first five peaks compatible with the zincblende selection rules are those of the FCC lattice, with Miller indices of the cubic structure equal to 111, 200, 220, 311, and 222. Then, by means of the Debye-Scherrer formula

$$\phi = 2 \sin^{-1} \left( \frac{\lambda}{2d} \right), \qquad \text{with } d = \frac{a}{\sqrt{h^2 + k^2 + l^2}},$$

we find $\phi_1 = 16.96°$, $\phi_2 = 19.61°$, $\phi_3 = 27.88°$, $\phi_4 = 32.81°$, $\phi_5 = 34.32°$.

3. The average sound velocity in the Debye approximation is

$$c_s = \left[ \frac{1}{3} \left( \frac{1}{c_l^3} + \frac{1}{c_{t1}^3} + \frac{1}{c_{t2}^3} \right) \right]^{-1/3} = 2035 \, \text{m} \cdot \text{s}^{-1}.$$

The Debye wave vector is $q_{\text{D}} = (6\pi^2 n)^{1/3} = 1.054 \times 10^{10} \, \text{m}^{-1}$, where $n = 4/a^3 = 1.977 \times 10^{28} \, \text{m}^{-3}$ is the density of Bravais lattice points. The Debye temperature is

$$\Theta_{\text{D}} = \frac{\hbar c_s q_{\text{D}}}{\kappa_B} = 163.8 \, \text{K}.$$

**Exercise 2.**

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

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

Then the coefficients of the linear combination of atomic orbitals within the tight binding method obey the set of linear equations

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

which have nontrivial solution only if

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

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 $k_y = \pm\frac{\pi}{a}$. These conditions correspond to the boundary of the first Brillouin zone. The values of the band energies are $E_+ = \varepsilon_{\mathrm{A}} = 5.75\,\mathrm{eV}$ and $E_- = \varepsilon_{\mathrm{B}} = 5.00\,\mathrm{eV}$.

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

$$E_{\pm} \approx \frac{\varepsilon_{\mathrm{A}} + \varepsilon_{\mathrm{B}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{2}\right)^2 + 16\gamma^2 - 4\gamma^2 a^2 k^2} \approx \frac{\varepsilon_{\mathrm{A}} + \varepsilon_{\mathrm{B}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{2}\right)^2 + 16\gamma^2} \left[1 - \frac{2\gamma^2 a^2 k^2}{\left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{2}\right)^2 + 16\gamma^2}\right].$$

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

$$E_{\pm} \approx \ldots \mp \frac{2\gamma^2 a^2 k^2}{\sqrt{\left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{2}\right)^2 + 16\gamma^2}},$$

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

$$m^* = \frac{\hbar^2 \sqrt{\left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{2}\right)^2 + 16\gamma^2}}{4\gamma^2 a^2} = \frac{\hbar^2}{\gamma a^2}\sqrt{1 + \left(\frac{\varepsilon_{\mathrm{A}} - \varepsilon_{\mathrm{B}}}{8\gamma}\right)^2} = \frac{\sqrt{65}\,\hbar^2}{8\gamma a^2} = 4.61 \times 10^{-31}\,\mathrm{kg} = 0.506\,m_0.$$