Written exam of Condensed Matter Physics - November 12th 2020 (dedicated session)
Profs. S. Caprara and A. Polimeni

Exercise 1. Consider the body centered tetragonal Bravais lattice whose conventional unit cell is displayed in Fig. 1(a). Describe the lattice as a tetragonal lattice with a two-site basis, taking as primitive vectors $\boldsymbol{a}_1 = a\,\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = a\,\hat{\boldsymbol{y}}$, and $\boldsymbol{a}_3 = c\,\hat{\boldsymbol{z}}$, where $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, $\hat{\boldsymbol{z}}$ are the unit vectors of the corresponding axes.

1. Introduce suitable basis vectors $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ that describe the body centered tetragonal lattice.

2. Find the primitive vectors of the reciprocal space, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$, then calculate the form factor $\mathcal{S}_{\boldsymbol{K}}$ (with $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + l\,\boldsymbol{b}_3$, for integer h, k, l) and determine the reciprocal lattice vectors of the tetragonal lattice that are not reciprocal lattice vectors of the body centered tetragonal lattice.

3. A solid with the given crystal structure is investigated by means of the Debye-Scherrer method, with an X-ray beam of wavelength $\lambda = 0.15\,\text{nm}$. Determine the lattice parameters a and c of the conventional unit cell knowing that the first diffraction peaks are found at scattering angles $\varphi = 2\vartheta = 18.17°$, $21.25°$, $27.27°$, $32.96°$, $33.67°$, $38.94°$ ...
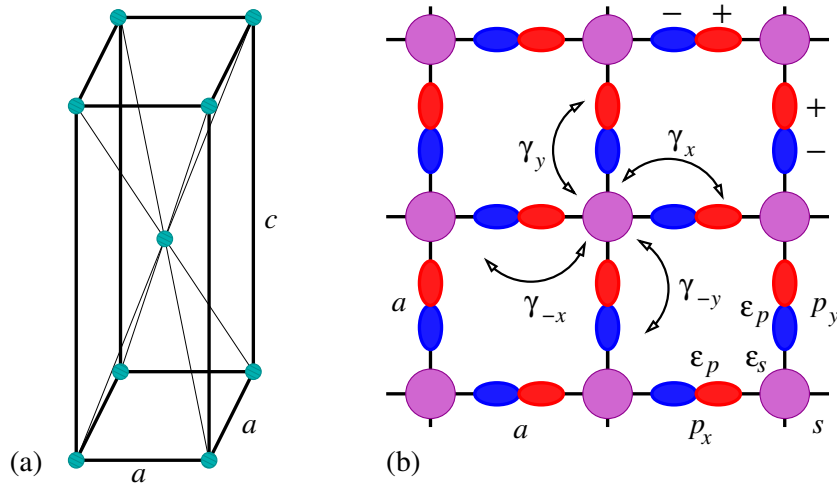

Fig. 1.

Exercise 2. Consider the two dimensional square Bravais lattice with a three-atom basis and lattice parameter $a = 0.4\,\text{nm}$ shown in Fig. 1(b) and assume that its electron states can be described within the tight binding model with attractive potential $\Delta U < 0$. The nodes of the lattice are occupied by atoms with external s orbitals, while half-way between two s orbitals in the $x\,(y)$ direction there are atoms with external $p_x\,(p_y)$ orbitals. The s orbitals are assigned a + sign, while the signs of the two lobes of each p orbital are assigned so that the positive (negative) lobe points in the positive (negative) direction of the corresponding axis. The nearest-neighbor transfer integrals $|\gamma_{\pm x\,(\pm y)}| = \gamma = 0.1\,\text{eV}$ are given [see Fig. 1(b)]. All other transfer integrals and all overlap integrals are negligible. The atomic levels are $\varepsilon_s = 0$ for s orbitals and $\varepsilon_p = 0.2\,\text{eV}$ for both p orbitals.

1. Determine the three branches of the dispersion law $\varepsilon_{s,\boldsymbol{k}}$ of Bloch electrons on the given lattice within the tight-binding approximation, with $s = 1, 2, 3$, $\boldsymbol{k} = (k_x, k_y)$ being the wave vector. The bands are labeled such that $\varepsilon_{1,\boldsymbol{k}} \leq \varepsilon_{2,\boldsymbol{k}} \leq \varepsilon_{3,\boldsymbol{k}}$. Show that the spectrum hosts a non-bonding (i.e., non dispersive) band.

2. In the situation when there are two electron per primitive cell, the system is a semiconductor. Determine the band gap, showing that it is located at the Γ point of the first Brillouin zone.

3. Considering only the two dispersive bands, determine the effective masses for electrons at the top of the valence band and for holes at the bottom of the conduction band.

[Useful constants and conversion factors: $\hbar = 1.055 \times 10^{-34}\,\text{J·s}$ (Planck's constant), $m_0 = 9.109 \times 10^{-31}\,\text{kg}$ (electron mass); $1\,\text{eV}$ corresponds to $1.602 \times 10^{-19}\,\text{J}$].

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Exercise 1.

1. One possible choice of the basis set is $\boldsymbol{d}_1 = \boldsymbol{0}$, $\boldsymbol{d}_2 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) + \frac{c}{2}\hat{\boldsymbol{z}}$.

2. By means of the formulas $\boldsymbol{b}_1 = 2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)/[\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)]$, etc., one finds $\boldsymbol{b}_1 = \frac{2\pi}{a}\hat{\boldsymbol{x}}$, $\boldsymbol{b}_2 = \frac{2\pi}{a}\hat{\boldsymbol{y}}$, $\boldsymbol{b}_3 = \frac{2\pi}{c}\hat{\boldsymbol{z}}$. The form factor is

$$\mathcal{S}_{\boldsymbol{K}} = \sum_{j=1,2} e^{i\boldsymbol{d}_j \cdot \boldsymbol{K}} = 1 + e^{i\pi(h+k+l)}.$$

Since $\mathcal{S}_{\boldsymbol{K}}$ vanishes whenever $h+k+l$ is odd, the corresponding reciprocal lattice vectors do not belong to the reciprocal lattice of the body centered tetragonal lattice.

3. The magnitude of a reciprocal lattice vector is

$$K \equiv |\boldsymbol{K}| = \frac{2\pi}{a}\sqrt{h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2},$$

when $h + k + l$ is even. Defining $\kappa = 2\pi/\lambda$, according to the Debye-Scherrer formula

$$\sin\frac{\varphi}{2} = \frac{K}{2\kappa} = \frac{\lambda}{2a}\sqrt{h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2}.$$

Now, the values for $l = 0$ correspond to the allowed families of lattice planes 110 and $200, 020$, so in the list one expects two angles that are in the ratio $\approx \sqrt{2}$. These are $27.27°$ and $38.94°$. Attributing the first angle to the family 110, one finds

$$\sin 13.365° = \frac{\lambda}{2a}\sqrt{2} \quad \rightarrow \quad a = \frac{\lambda}{2\sin 13.365°}\sqrt{2} \approx 0.46\,\text{nm}.$$

Now, the first peak, must correspond, either to the 002 or to the $101, 011$ families. The first possibility gives

$$\sin 9.085° = \frac{\lambda}{c} \quad \rightarrow \quad c = \frac{\lambda}{\sin 9.085°} \approx 0.95\,\text{nm}.$$

These two values for a and c match all the other angles. The families of lattice planes that correspond to the various angles are 002; $101, 011$; 110; 112; $103, 013$; $200, 020$; ...

Exercise 2.

1. Calling b_s, b_x, b_y the coefficients of the linear combination of s, p_x, p_y orbitals, respectively, within the tight-binding method one has to solve the following homogeneous system of three linear equations:

$$\begin{cases} (\varepsilon_s - \varepsilon_{\boldsymbol{k}})b_s + \gamma\left(e^{i\,a\,k_x/2} - e^{-i\,a\,k_x/2}\right)b_x + \gamma\left(e^{i\,a\,k_y/2} - e^{-i\,a\,k_y/2}\right)b_y = 0 \\[2mm] (\varepsilon_p - \varepsilon_{\boldsymbol{k}})b_x - \gamma\left(e^{i\,a\,k_x/2} - e^{-i\,a\,k_x/2}\right)b_s = 0 \\[2mm] (\varepsilon_p - \varepsilon_{\boldsymbol{k}})b_y - \gamma\left(e^{i\,a\,k_y/2} - e^{-i\,a\,k_y/2}\right)b_s = 0 \end{cases}$$

that has nontrivial solutions only when the energy $\varepsilon_{\boldsymbol{k}}$ equals one of the three eigenvalues

$$\varepsilon_{1,\boldsymbol{k}} = \frac{\varepsilon_p + \varepsilon_s}{2} - \sqrt{\left(\frac{\varepsilon_p - \varepsilon_s}{2}\right)^2 + 4\gamma^2 s_{\boldsymbol{k}}^2}, \qquad \varepsilon_{2,\boldsymbol{k}} = \varepsilon_p, \qquad \varepsilon_{3,\boldsymbol{k}} = \frac{\varepsilon_p + \varepsilon_s}{2} + \sqrt{\left(\frac{\varepsilon_p - \varepsilon_s}{2}\right)^2 + 4\gamma^2 s_{\boldsymbol{k}}^2}.$$

with $s_{\boldsymbol{k}}^2 \equiv \sin^2\frac{a\,k_x}{2} + \sin^2\frac{a\,k_y}{2}$. The non-bonding band $\varepsilon_{2,\boldsymbol{k}}$ corresponds to a linear combination of p orbitals that does not bind to the s orbital.

2. Since the dispersion term $s_{\boldsymbol{k}}^2$ is minimum ($= 0$) at the Γ point, the band $\varepsilon_{1,\boldsymbol{k}}$ attains its maximum value, ε_s, at this point. Similarly, the band $\varepsilon_{3,\boldsymbol{k}}$ attains its minimum value, ε_p, at the Γ point. Thus, the gap is $E_g = \varepsilon_p - \varepsilon_s = 0.2\,\mathrm{eV}$.

3. Expanding the bands $\varepsilon_{1,\boldsymbol{k}}$ and $\varepsilon_{3,\boldsymbol{k}}$ around the Γ point, where $s_{\boldsymbol{k}}^2 \approx \frac{a^2 k^2}{4}$, with $k^2 \equiv k_x^2 + k_y^2$, one finds

$$\varepsilon_{1,\boldsymbol{k}} \approx \varepsilon_s - \frac{4\gamma^2 s_{\boldsymbol{k}}^2}{\varepsilon_p - \varepsilon_s} \approx \varepsilon_s - \frac{2\gamma^2 a^2}{\varepsilon_p - \varepsilon_s}\frac{k^2}{2}, \qquad \varepsilon_{1,\boldsymbol{k}} \approx \varepsilon_p + \frac{4\gamma^2 s_{\boldsymbol{k}}^2}{\varepsilon_p - \varepsilon_s} \approx \varepsilon_p + \frac{2\gamma^2 a^2}{\varepsilon_p - \varepsilon_s}\frac{k^2}{2},$$

the masses of electrons and holes are the same

$$m_e = m_h = \frac{\hbar^2(\varepsilon_p - \varepsilon_s)}{2\gamma^2 a^2} = 4.34 \times 10^{-30}\,\mathrm{kg} = 4.76\,m_0.$$