Written exam of Condensed Matter Physics - June 18th 2019
Profs. S. Caprara and A. Polimeni

Exercise 1: X-ray diffraction.

Consider a crystal described as an orthorhombic Bravais lattice with lattice parameters $a = \frac{2}{3}s$, $b = s$, $c = \frac{3}{2}s$, where the length scale s is assigned [see Fig. 1 (a)]. The structure of the crystal is investigated by means of the Debye-Scherrer method, with a radiation of wavelength λ.

1. Having adopted the fundamental vectors $\boldsymbol{a}_1 = (a, 0, 0) = (\frac{2}{3}s, 0, 0)$, $\boldsymbol{a}_2 = (0, b, 0) = (0, s, 0)$, and $\boldsymbol{a}_3 = (0, 0, c) = (0, 0, \frac{3}{2}s)$, determine the reciprocal lattice vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ of the given lattice, for any given s.

2. Determine the families of lattice planes (hkl) that produce the first ten observed peaks, in order of increasing magnitude of the related reciprocal lattice vectors.

3. Determine the ratio λ/s, knowing that the first peak is observed at an angle $\phi_1 = 2\theta_1 = 16°$.

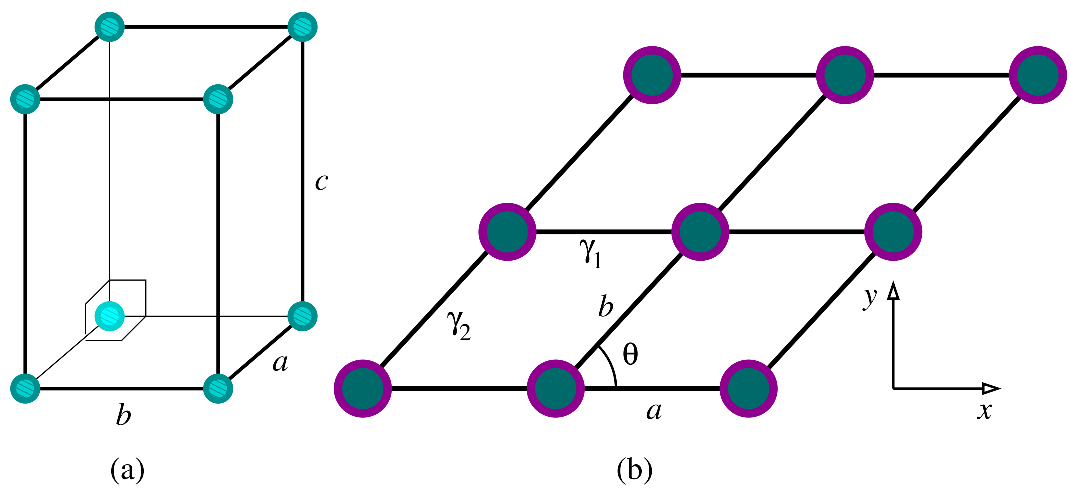

Fig. 1.

Exercise 2: Tight binding.

Consider the two-dimensional crystal described by the monoclinic Bravais lattice shown in Fig. 1 (b). The lattice sites host s orbitals, the two transfer integrals γ_1 and γ_2 are assigned, all the other transfer integrals and all the overlap integrals can be neglected. Here, the standard notation $\gamma_i \equiv \gamma(\boldsymbol{R}_i) = -\int \mathrm{d}\boldsymbol{r}\, \phi_s(\boldsymbol{r})\Delta U(\boldsymbol{r})\phi_s(\boldsymbol{r} - \boldsymbol{R}_i)$ is adopted. The energy level of the atomic s orbital is E_s, and $\beta \equiv \gamma(\boldsymbol{R} = 0)$ is the shift of the atomic level.

1. Determine the tight-binding band dispersion for Bloch electrons in the given crystal.

2. Let now $a = 0.2\,\mathrm{nm}$, $b = 0.4\,\mathrm{nm}$, $\theta = 50° \approx 0.873\,\mathrm{rad}$, $\gamma_1 = 0.4\,\mathrm{eV}$, and $\gamma_2 = 0.2\,\mathrm{eV}$. Determine the inverse effective mass tensor at the Γ point of the first Brillouin zone, m^{-1}_{ij}, with $i = x, y$ and $j = x, y$.

3. Assuming that each atom contributes one electron, calculate the electron density n (number of electrons per unit surface) in the given crystal.

[Note that $1\,\mathrm{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$; the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$; the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$].

Solution of the written exam
Profs. S. Caprara and A. Polimeni

Exercise 1.

1. The volume of the unit cell is $\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = s^3$. The reciprocal lattice vectors are

$$\boldsymbol{b}_1 = 2\pi \frac{(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{3\pi}{s}(1,0,0), \qquad \boldsymbol{b}_2 = 2\pi \frac{(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{s}(0,1,0), \qquad \boldsymbol{b}_3 = 2\pi \frac{(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{4\pi}{3s}(0,0,1).$$

2. The magnitude of the reciprocal lattice vector $\boldsymbol{K} = h\,\boldsymbol{b}_1 + k\,\boldsymbol{b}_2 + l\,\boldsymbol{b}_3 = \frac{\pi}{3s}(9h, 6k, 4l)$ is $K = |\boldsymbol{K}| = \frac{\pi}{3s}\sqrt{81\,h^2 + 36\,k^2 + 16\,l^2}$. The magnitude of the wave vector of the radiation is $\kappa = \frac{2\pi}{\lambda}$

The peaks measured by means of the Debye-Scherrer technique are found at scattering angles ϕ that must obey the condition

$$\sin\frac{\phi}{2} = \frac{K}{2\kappa} = \frac{\lambda}{12s}\sqrt{81\,h^2 + 36\,k^2 + 16\,l^2} \equiv \frac{\lambda}{12s}\sqrt{N_{hkl}}.$$

where, hereafter, $N_{hkl} \equiv 81\,h^2 + 36\,k^2 + 16\,l^2$. From the expression of K it is evident that increasing N_{hkl} corresponds to increasing K. The shortest reciprocal lattice vector corresponds to the family of planes (001), for which $N_{001} = 16$; then comes the family (010), with $N_{010} = 36$; the third peak corresponds to the family (011), with $N_{011} = 52$; then comes the family (002), with $N_{002} = 64$; the fifth peak corresponds to the family (100), with $N_{100} = 81$; then comes the family (101), with $N_{101} = 97$; the seventh peak corresponds to the family (012), with $N_{012} = 100$; then comes the family (110), with $N_{110} = 117$; the ninth peak corresponds to the family (111), with $N_{111} = 133$; the tenth peak corresponds to two inequivalent families of lattice planes, (020) and (003), that are indistinguishable by means of the Debye-Scherrer technique, as they both give $N_{020} = N_{003} = 144$.

3. The first peak corresponds to $N_{001} = 16$. Then

$$\sin\frac{\phi_1}{2} = \frac{\lambda}{12s}\sqrt{N_{001}} = \frac{\lambda}{3s} \quad \Rightarrow \quad \frac{\lambda}{s} = 3\sin\frac{\phi_1}{2} \approx 0.418.$$

Exercise 2.

1. Denoting the lattice vectors with $\boldsymbol{R}_1 \equiv (a, 0)$ and $\boldsymbol{R}_2 \equiv (b\cos\theta, b\sin\theta)$, the tight-binding band dispersion is

$$\begin{aligned}\varepsilon_{\boldsymbol{k}} &= E_s - \beta - 2\gamma_1 \cos(\boldsymbol{R}_1 \cdot \boldsymbol{k}) - 2\gamma_2 \cos(\boldsymbol{R}_2 \cdot \boldsymbol{k}) \\ &= E_s - \beta - 2\gamma_1 \cos(ak_x) - 2\gamma_2 \cos(b\cos\theta k_x + b\sin\theta k_y)\end{aligned}$$

2. Expanding the band dispersion near the Γ point of the first Brillouin zone one finds

$$\varepsilon_{\boldsymbol{k}} \approx E_s - \beta - 2\gamma_1 - 2\gamma_2 + (\gamma_1 a^2 + \gamma_2 b^2 \cos^2\theta)k_x^2 + \gamma_2 b^2 \sin^2\theta\, k_y^2 + 2\gamma_2 b^2 \sin\theta\cos\theta\, k_x k_y.$$

Comparing with the expression

$$\varepsilon_{\boldsymbol{k}} = \text{const.} + \frac{\hbar^2}{2}\sum_{ij=x,y} m_{ij}^{-1} k_i k_j,$$

one finds

$$m_{xx}^{-1} = \frac{2}{\hbar^2}(\gamma_1 a^2 + \gamma_2 b^2 \cos^2\theta), \qquad m_{yy}^{-1} = \frac{2}{\hbar^2}\gamma_2 b^2 \sin^2\theta, \qquad m_{xy}^{-1} = m_{yx}^{-1} = \frac{2}{\hbar^2}\gamma_2 b^2 \sin\theta\cos\theta,$$

consistent with the monoclinic symmetry. For the given set of parametrs,

$$m_{xx}^{-1} = 8.42 \times 10^{29}\,\text{kg}^{-1} = 0.766\, m_0^{-1}, \qquad m_{yy}^{-1} = 5.42 \times 10^{29}\,\text{kg}^{-1} = 0.492\, m_0^{-1},$$

$$m_{xy}^{-1} = m_{yx}^{-1} = 4.54 \times 10^{29}\,\mathrm{kg}^{-1} = 0.414\, m_0^{-1}.$$

3. There is one atom per unit cell, and each atom contributes one electron, therefore

$$n = \frac{1}{ab\sin\theta} \approx 1.63 \times 10^{19}\,\mathrm{m}^{-2}.$$