Written exam for the dedicated call of Condensed Matter Physics - November 22nd 2021
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Exercise 1: X ray scattering.

The 5th diffraction peak of germanium in a powder diffraction experiment occurs at $\phi = 69.27^\circ$ using an x-ray beam with wavelength $\lambda = 1.476 \times 10^{-10}\,\mathrm{m}$ (see left panel in Fig. 1). Germanium is a face-centered cubic lattice with two-atom basis, one displaced with respect to the other by $\boldsymbol{d} = \frac{1}{4}(a, a, a)$ (see central panel in Fig. 1).

1. Determine the atomic density ρ_{at} of germanium.

2. Suppose that the experiment described above is performed with an incident beam consisting of neutrons. What must the neutron velocity be in order to produce reflections at the same angles as those produced by x-rays?

3. The sound velocity in germanium is $c_l = 5130\,\mathrm{m/s}$ for longitudinal mode and $c_t = 3360\,\mathrm{m/s}$ for transverse modes. Determine the average sound velocity c_{D} of germanium within the Debye model and the corresponding Debye temperature Θ_{D}.

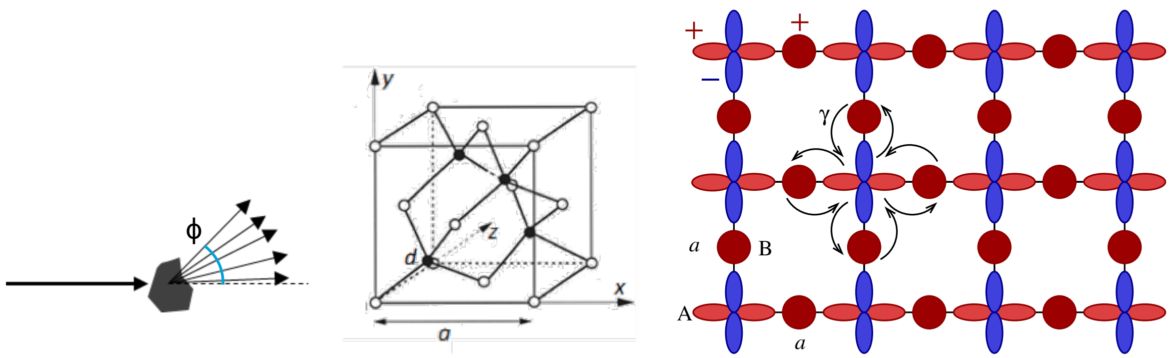

Fig. 1.

Exercise 2: Tight binding.

Consider a two-dimensional crystal that can be described as a square Bravais lattice with side of the primitive cell $a = 0.5\,\mathrm{nm}$, hosting a compound with chemical formula AB_2 (see right panel in Fig. 1). Each B atom is exactly halfway between two A atoms. The A atoms contribute to the formation of the relevant bands with $d_{x^2-y^2}$ orbitals, while the B atoms contribute with s orbitals. The s orbitals are assigned a positive sign, the sign of the $d_{x^2-y^2}$ orbitals is positive for the lobes along the x axis and negative for the lobes along the y axis. The atomic energy of the corresponding orbitals is $E_{\mathrm{A}} = 1.5\,\mathrm{eV}$ and $E_{\mathrm{B}} = 1.0\,\mathrm{eV}$ for A and B atoms, respectively. Assume that the bands can be described within the tight binding approximation with $\Delta U < 0$ and consider only the nearest-neighbor transfer integral, with absolute value $\gamma = 0.25\,\mathrm{eV}$ between A and B atoms, while neglecting all other transfer integrals, all overlap integrals, and assuming the β integrals to be zero for simplicity.

1. Assign the correct sign to the transfer integrals between $d_{x^2-y^2}$ and s orbitals along the x and y axis and determine the tight-binding dispersion law $\varepsilon_{\alpha,\boldsymbol{k}}$, with wavevector $\boldsymbol{k} = (k_x, k_y)$ and $\alpha = 1, 2, 3$, for the three bands that are formed after the hybridization of the orbitals of the A and B atoms. Number the three bands in ascending order, and verify that there is a flat band with energy E_{B}.

2. Determine the value of the band gap E_g and its location in $\boldsymbol{k}$ space.

3. Considering only the dispersive bands, determine the values of the elements of the effective mass tensors for electrons near the bottom of the conduction band and for holes near the top of the valence band, m^{e}_{ij} and m^{h}_{ij}, respectively, with $i = x, y$, $j = x, y$.

[Note that the neutron mass is $m_{\mathrm{n}} = 1.67 \times 10^{-27}\,\mathrm{kg}$; the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\mathrm{J{\cdot}s}$; the Boltzmann constant is $\kappa_{\mathrm{B}} = 1.38 \times 10^{-23}\,\mathrm{J/K}$; $1\,\mathrm{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$; the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\mathrm{kg}$].

Solution of the written exam
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Exercise 1.

1. We know that $\rho_{\rm at} = \frac{8}{a^3}$. The 5th reflection corresponds to a plane spacing $d = \lambda/(2\sin\theta)$, where $d = a\sqrt{h^2+k^2+l^2}$ with $(h,k,l) = (331)$ according to the diamond selection rules (see Fig. 2). Since $\phi = 2\theta = 69.27°$, we obtain $d = 1.299 \times 10^{-10}$ m and $a = 5.66 \times 10^{-10}$ m. Thus, $\rho_{\rm at} = 4.412 \times 10^{28}\,{\rm m}^{-3}$.

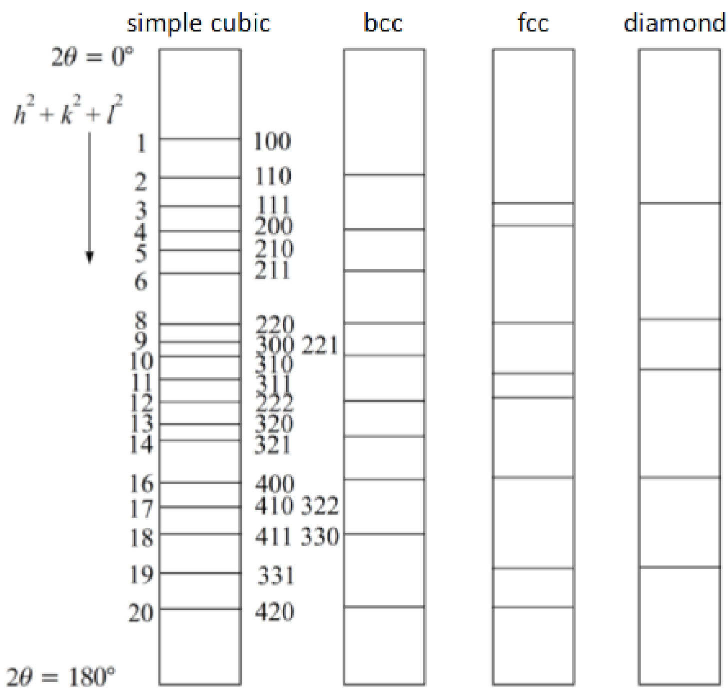

Fig. 2.

2. To have the same scattering angles, the wavelength of the neutron must be equal to the wavelength of the x-ray beam, hence, using De Broglie formula (in the non relativistic limit),

$$v = \frac{h}{m_{\rm n}\lambda} = \frac{2\pi\hbar}{m_{\rm n}\lambda} = 2.68 \times 10^3\,{\rm m/s}.$$

3. The average sound velocity is such that

$$\frac{1}{c_{\rm D}^3} = \frac{1}{3}\left(\frac{1}{c_l^3} + \frac{2}{c_t^3}\right),$$

hence $c_{\rm D} = 3681\,{\rm m/s}$. The Debye wavevector is $q_{\rm D} = (6\pi^2 n)^{1/3}$ where $n = 4/a^3$ is the density of Bravais lattice points, hence $q_{\rm D} = 1.09 \times 10^{10}\,{\rm m}^{-1}$. Finally, the Debye temperature is

$$\Theta_{\rm D} = \frac{\hbar c_{\rm D} q_{\rm D}}{\kappa_{\rm B}} = 307.4\,{\rm K}.$$

Exercise 2.

1. The transfer integrals are positive along the x axis and negative along the y axis. Calling b_d, b_x, b_y the coefficients of the linear combination of d orbitals of A atoms, and of s orbitals of B atoms along the x and y axis, respectively, within the tight-binding method one has to solve the following homogeneous system of three linear equations:

$$\begin{cases} (E_{\mathrm{A}} - \varepsilon_{\boldsymbol{k}})b_d - \gamma\left(\mathrm{e}^{\mathrm{i}\,a\,k_x/2} + \mathrm{e}^{-\mathrm{i}\,a\,k_x/2}\right)b_x + \gamma\left(\mathrm{e}^{\mathrm{i}\,a\,k_y/2} + \mathrm{e}^{-\mathrm{i}\,a\,k_y/2}\right)b_y = 0 \\ (E_{\mathrm{B}} - \varepsilon_{\boldsymbol{k}})b_x - \gamma\left(\mathrm{e}^{\mathrm{i}\,a\,k_x/2} + \mathrm{e}^{-\mathrm{i}\,a\,k_x/2}\right)b_d = 0 \\ (E_{\mathrm{B}} - \varepsilon_{\boldsymbol{k}})b_y + \gamma\left(\mathrm{e}^{\mathrm{i}\,a\,k_y/2} + \mathrm{e}^{-\mathrm{i}\,a\,k_y/2}\right)b_d = 0 \end{cases}$$

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

$$\varepsilon_{1,\boldsymbol{k}} = \frac{E_{\mathrm{A}} + E_{\mathrm{B}}}{2} - \sqrt{\left(\frac{E_{\mathrm{A}} - E_{\mathrm{B}}}{2}\right)^2 + 4\gamma^2 c_{\boldsymbol{k}}^2}, \qquad \varepsilon_{2,\boldsymbol{k}} = E_{\mathrm{B}}, \qquad \varepsilon_{3,\boldsymbol{k}} = \frac{E_{\mathrm{A}} + E_{\mathrm{B}}}{2} + \sqrt{\left(\frac{E_{\mathrm{A}} - E_{\mathrm{B}}}{2}\right)^2 + 4\gamma^2 c_{\boldsymbol{k}}^2}.$$

with $c_{\boldsymbol{k}}^2 \equiv \cos^2\left(\frac{a\,k_x}{2}\right) + \cos^2\left(\frac{a\,k_y}{2}\right)$. The flat band $\varepsilon_{2,\boldsymbol{k}}$ corresponds to a linear combination of s orbitals of the B atoms that does not bind to the $d_{x^2-y^2}$ orbital of the A atom.
2. Since the dispersion term $c_{\boldsymbol{k}}^2$ is minimum $(= 0)$ at the $M = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$ point of the first Brillouin zone, the band $\varepsilon_{1,\boldsymbol{k}}$ attains its maximum value, E_{B}, at this point. Similarly, the band $\varepsilon_{3,\boldsymbol{k}}$ attains its minimum value, E_{A}, at this point. Thus, the gap is $E_g = E_{\mathrm{A}} - E_{\mathrm{B}} = 0.5\,\mathrm{eV}$.

3. Expanding the bands $\varepsilon_{1,\boldsymbol{k}}$ and $\varepsilon_{3,\boldsymbol{k}}$ around the M point, where $c_{\boldsymbol{k}}^2 \approx \frac{1}{4}a^2\delta k^2$, with $\delta k^2 \equiv \delta k_x^2 + \delta k_y^2 \equiv \left(k_x - \frac{\pi}{a}\right)^2 + \left(k_y - \frac{\pi}{a}\right)^2$, one finds

$$\varepsilon_{1,\boldsymbol{k}} \approx E_{\mathrm{B}} - \frac{4\gamma^2 c_{\boldsymbol{k}}^2}{E_{\mathrm{A}} - E_{\mathrm{B}}} \approx E_{\mathrm{B}} - \frac{2\gamma^2 a^2}{E_{\mathrm{A}} - E_{\mathrm{B}}}\frac{\delta k^2}{2}, \qquad \varepsilon_{3,\boldsymbol{k}} \approx E_{\mathrm{A}} + \frac{4\gamma^2 c_{\boldsymbol{k}}^2}{E_{\mathrm{A}} - E_{\mathrm{B}}} \approx E_{\mathrm{A}} + \frac{2\gamma^2 a^2}{E_{\mathrm{A}} - E_{\mathrm{B}}}\frac{\delta k^2}{2},$$

hence the mass tensors are diagonal at the M point, $m_{ij}^{\mathrm{e}} = m^{\mathrm{e}}\delta_{ij}$ and $m_{ij}^{\mathrm{h}} = m^{\mathrm{h}}\delta_{ij}$, where δ_{ij} is the Kronecker symbol and

$$m^{\mathrm{e}} = m^{\mathrm{h}} = \frac{\hbar^2(E_{\mathrm{A}} - E_{\mathrm{B}})}{2\gamma^2 a^2} = 1.11 \times 10^{-30}\,\mathrm{kg} = 1.22\,m_0.$$