Written exam of Condensed Matter Physics - february 7th 2022
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Exercise 1. Two binary crystals, AB and CD, have a lattice with cubic symmetry, with the A and B atoms forming a basis in the former, and the C and D atoms forming a basis in the latter. When measuring the X-ray diffraction pattern of the two samples using the powder method by a radiation with wavelength $\lambda = 0.154056\,\text{nm}$, seven diffraction peaks are obtained for each sample, with the scattering angle 2θ as shown below:

$$\text{AB)}\ 2\theta\,(^\circ) = 25.2078,\ 35.94916,\ 44.41354,\ 51.75128,\ 58.40944,\ 64.62032,\ 76.22245;$$

$$\text{CD)}\ 2\theta\,(^\circ) = 36.90612,\ 42.87606,\ 62.2474,\ 74.6167,\ 78.5518,\ 93.93879,\ 105.60895.$$

1. [8 points] For each of the two compounds, identify the crystal structure, label the diffraction peaks using the Miller indexing of the simple cubic lattice, and compute the average lattice parameter a of the cubic cell.

2. [4 points] Indicate which of the above peaks would disappear if the atoms A and B in the AB sample, or C and D in the CD sample, were the same, with one atom positioned in the origin $(0,0,0)$ and the other atom positioned at $a\,\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$.

3. [3 points] Evaluate the Debye wavevector q_D, associated to the acoustic modes only, for the two crystals.

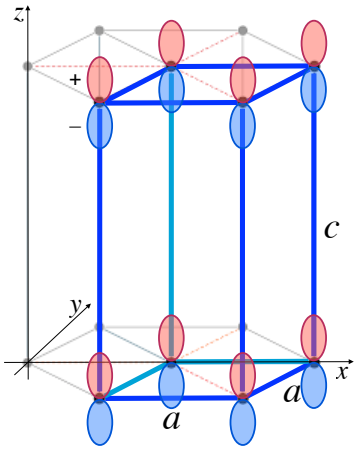

Fig. 1.

Exercise 2. A hexagonal lattice with lattice parameters $a = 0.425\,\text{nm}$ and $c = 0.625\,\text{nm}$ (see Fig. 1, where the conventional unit cell is shown and a primitive cell is highlighted with thicker lines) hosts an element with p_z valence orbitals (only the orbitals at the vertices of the primitive cell are shown, not to overcrowd the figure). The convention for the signs of the two lobes of the p_z orbitals is the one adopted in Fig. 1. Assume that the electron states can be described within a tight-binding approximation, with attractive lattice potential $\Delta U(\boldsymbol{r}) < 0$. Consider only the nearest-neighbors transfer integrals in the basal plane, $|\gamma_a| = 0.2\,\text{eV}$, and along the c axis, $|\gamma_c| = 0.1\,\text{eV}$. All other transfer integrals and all overlap integrals are negligible. The atomic energy of the p_z orbitals is $E_p = -6.1\,\text{eV}$ and the tight-binding shift is $\beta = 0.4\,\text{eV}$.

1. [3 points] Assign the correct sign to γ_a and γ_c, motivating your answer.

2. [5 points] Determine the tight-binding dispersion law $E_{\boldsymbol{k}}$, where $\boldsymbol{k} = (k_x, k_y, k_z)$ is the Bloch wave vector.

3. [7 points] Determine the values of the band energy $E_{\boldsymbol{k}}$ and of the elements of the mass tensor m_{ij}, $i,j = x,y,z$, at the Γ point of the first Brillouin zone.

[Useful constants and conversion factors: $\hbar = 1.055\times10^{-34}\,\text{J·s}$ (Planck's constant), 1 eV corresponds to $1.602\times10^{-19}\,\text{J}$, the free electron mass is $m_0 = 9.109\times10^{-31}\,\text{kg}$.].

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Exercise 1.

1. AB is a simple cubic lattice, as shown in the table below:

n	2θ (°)	d (nm)	$(d_1/d_n)^2$	(hkl)	$(h_n^2+k_n^2+l_n^2)/(h_1^2+k_1^2+l_1^2)$	a (nm)
1	25.2078	0.353	1	100	1	0.3530
2	35.94916	0.24961	2	110	2	0.3530
3	44.41354	0.2038	3	111	3	0.3530
4	51.75128	0.1765	4	200	4	0.3530
5	58.40944	0.15787	5	210	5	0.3530
6	64.62032	0.14411	6	211	6	0.3530
7	76.22245	0.1248	8	220	8	0.3530

where $d = \lambda/(2\sin\theta)$ and $a = d\sqrt{h^2+k^2+l^2}$. From the table, we deduce $a = 0.3530\,\text{nm}$. CD is a face centered cubic lattice, as shown in the table below:

n	2θ (°)	d (nm)	$(d_1/d_n)^2$	(hkl)	$(h_n^2+k_n^2+l_n^2)/(h_1^2+k_1^2+l_1^2)$	a (nm)
1	36.90612	0.24335	1	111	1	0.4215
2	42.87606	0.21075	1.3333	200	1.33333	0.4215
3	62.2474	0.14902	2.6666	220	2.66667	0.4215
4	74.6167	0.12709	3.66657	311	3.66667	0.4215
5	78.5518	0.12168	3.9999	222	4	0.4215
6	93.93879	0.10538	5.3332	400	5.33333	0.4215
7	105.60895	0.0967	6.33317	331	6.33333	0.4215

where again $d = \lambda/(2\sin\theta)$ and $a = d\sqrt{h^2+k^2+l^2}$. From the table, we deduce $a = 0.4215\,\text{nm}$.

2. If we set the basis as $\boldsymbol{\rho}_1 = (0,0,0)$ and $\boldsymbol{\rho}_2 = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$, and take the reciprocal lattice vectors of the simple cubic, $\boldsymbol{G} = h\boldsymbol{g}_1 + k\boldsymbol{g}_2 + l\boldsymbol{g}_3$, where $\boldsymbol{g}_1 = \frac{2\pi}{a}(1,0,0)$, $\boldsymbol{g}_2 = \frac{2\pi}{a}(0,1,0)$, $\boldsymbol{g}_3 = \frac{2\pi}{a}(0,0,1)$, the basis structure factor is $\mathcal{S}_{\boldsymbol{G}} = 1 + \mathrm{e}^{-\mathrm{i}\pi(h+k+l)}$. This factor is zero for odd $h+k+l$. For the AB lattice, the disappearing peaks are those labeled as $n = 1$, 3, and 5. For the CD lattice, the disappearing peaks are $n = 1$, 4, and 7.

3. The Debye wavevector of the sound modes is $q_\text{D} = (6\pi^2 n)^{1/3}$, where n is the density of Bravais lattice points. For the AB sample, $n = 1/a^3$ and $q_\text{D} = 11.04\,\text{nm}^{-1}$. For the CD sample, $n = 4/a^3$ and $q_\text{D} = 14.68\,\text{nm}^{-1}$.

Exercise 2.

1. Since neighboring lobes of the p_z orbitals in the basal plane have the same sign, $\gamma_a > 0$; similarly, since neighboring lobes of the p_z orbitals along the c axis have opposite signs, $\gamma_c < 0$. In the following, let us put $\tilde{\gamma}_c = -\gamma_c = |\gamma_c| > 0$.

2. Let $\boldsymbol{R}_a = (a, 0, 0)$, $\boldsymbol{R}_\pm = \left(\frac{a}{2}, \pm\frac{a\sqrt{3}}{2}, 0\right)$, and $\boldsymbol{R}_c = (0, 0, c)$, then we have

$$E_{\boldsymbol{k}} = E_p - \beta - \sum_{\boldsymbol{R}} \gamma(\boldsymbol{R})\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} = E_p - \beta - \gamma_a \sum_{\substack{\boldsymbol{R}=\pm\boldsymbol{R}_a,\\ \pm\boldsymbol{R}_\pm}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} - \gamma_c \sum_{\boldsymbol{R}=\pm\boldsymbol{R}_c} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$= E_p - \beta - 2\gamma_a \left\{\cos(k_x a) + \cos\left[\frac{a}{2}(k_x + \sqrt{3}k_y)\right] + \cos\left[\frac{a}{2}(k_x - \sqrt{3}k_y)\right]\right\} - 2\gamma_c \cos(k_z c)$$

$$= E_s - \beta - 2\gamma_a \left[\cos(k_x a) + 2\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\right] + 2\tilde{\gamma}_c \cos(k_z c).$$

3. At the Γ point $E_{\boldsymbol{k}=(0,0,0)} = E_p - \beta - 6\gamma_a + 2\tilde{\gamma}_c = -7.5\,\mathrm{eV}$. Expanding the band dispersion around the Γ point, we find

$$E_{\boldsymbol{k}} \approx E_s - \beta - 6\gamma_a + 2\tilde{\gamma}_c + \frac{3}{2}\gamma_a a^2 \left(k_x^2 + k_y^2\right) - \tilde{\gamma}_c c^2 k_z^2,$$

hence the mass tensor is diagonal, the only nonzero elements being

$$m_{xx} = m_{yy} = \frac{\hbar^2}{3\gamma_a a^2} = 6.41 \times 10^{-31}\,\mathrm{kg} = 0.704\, m_0,$$

$$m_{zz} = -\frac{\hbar^2}{2\tilde{\gamma}_c c^2} = -8.89 \times 10^{-31}\,\mathrm{kg} = -0.976\, m_0.$$

This is a saddle point of the band dispersion.