Written exam of Condensed Matter Physics - September 9th 2021
Profs. S. Caprara and A. Polimeni

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

A sample made of silver (Ag, featuring a cubic symmetry) is ground into powder and subjected to a Debye-Scherrer diffraction experiment employing X rays of wavelength $\lambda = 0.154\,\text{nm}$. The following set of reflections expressed as $2\theta = 38.257°$, $44.467°$, $64.702°$, $77.727°$, $81.896°$ is observed.

1. Determine the nature (simple, FCC, BCC) and the lattice constant a and of the cubic cell of silver. [**7 points**].

2. Calculate the Debye temperature Θ_D of the sound modes of silver, and verify that at $T = 20\,\text{K}$ the Debye approximation for the determination of the lattice specific heat is reasonable, knowing that the average sound velocity is $v_s = 2.5 \times 10^5\,\text{cm/s}$. [**4 points**].

3. Determine the lattice specific heat c_V^ph of silver at $T = 20\,\text{K}$. [**4 points**].

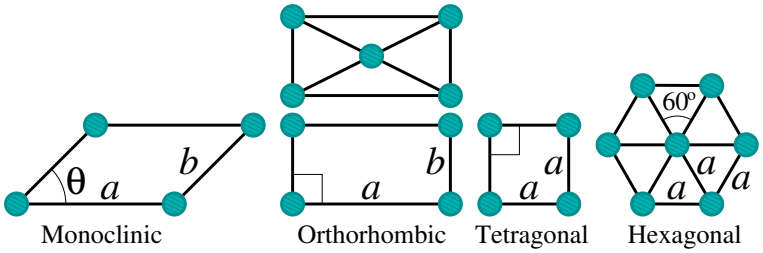

Fig. 1.

Exercise 2: Bloch electrons [15 points].

Consider a two-dimensional crystal, whose conduction and valence bands [$E_\text{c}(\boldsymbol{k})$ and $E_\text{v}(\boldsymbol{k})$, respectively] have the following expressions:

$$E_\text{c}(\boldsymbol{k}) = A - B\left[\cos(a\,k_x) + \cos(b\,k_y) - \frac{1}{5}\cos(a\,k_x)\cos(b\,k_y)\right],$$

$$E_\text{v}(\boldsymbol{k}) = C\left[\cos(a\,k_x) + \cos(b\,k_y) - \frac{1}{4}\cos(a\,k_x)\cos(b\,k_y)\right],$$

where $\boldsymbol{k} = (k_x, k_y)$ is the two-dimensional Bloch wavevector, $a = 0.5\,\text{nm}$, $b = 0.4\,\text{nm}$, $A = 2.0\,\text{eV}$, $B = 0.5\,\text{eV}$, and $C = 0.4\,\text{eV}$. The electron filling is such that the valence band is completely filled and the conduction band is empty at $T = 0$.

1. Considering the symmetries of the electron spectrum, deduce the two-dimensional crystal family (monoclinic, orthorhombic, tetragonal, or hexagonal, see Fig. 1) to which the given crystal belongs, motivating your answer [**2 points**].

2. Calculate the numerical value of the gap E_g between the valence and the conduction band and determine whether the gap is direct or indirect [**4 points**].

3. Draw the dispersion curves in the ΓX $[(0,0) \to (\pi/a, 0)]$ and ΓS $[(0,0) \to (\pi/a, \pi/b)]$ directions, marking on the energy axis the position of the extremal points of the two bands (in the given direction) [**4 points**].

4. Determine the numerical values of the elements of the mass tensor for electrons at the minimum of the conduction band (m^c_{ij}, with $i = x, y$, $j = x, y$) and for holes at the maximum of the valence band (m^v_{ij}, with $i = x, y$, $j = x, y$) [**5 points**].

[Note that 1 eV corresponds to an energy of 1.602×10^{-19} J; the Planck constant is $\hbar = 1.055\times10^{-34}$ J·s; the Boltzmann constant is $\kappa_B = 1.381 \times 10^{-23}\,\text{J·K}^{-1}$; the free electron mass is $m_0 = 9.109 \times 10^{-31}$ kg].

Solution of the written exam
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Exercise 1.

1. Using the usual analysis of the Debye-Scherrer experiments, one obtains the following table

2θ (°)	*d* (nm)	1/d² norm.	integer	hkl	a (nm)
38.257	0.23498	1	3	111	0.407
44.467	0.2035	1.33334	4.00001	200	0.407
64.702	0.1439	2.66659	7.99977	220	0.407
77.727	0.12272	3.66658	10.99974	311	0.407
81.896	0.11749	3.99998	11.99993	222	0.407

where $d = \lambda/2\sin\theta$, and $a = d\sqrt{h^2+k^2+l^2}$, whence $a = 0.407\,\mathrm{nm}$. From the values of the Miller indices hkl it is evident that silver has a FCC conventional unit cell.

2. We estimate the Debye temperature using $k_\mathrm{D} = \sqrt[3]{6\pi^2 n}$ with $n = 4/a^3 = 5.933\times10^{28}\,\mathrm{m}^{-3}$, obtaining $k_\mathrm{D} = 1.520\times10^{10}\,\mathrm{m}^{-1}$. Then, $\Theta_\mathrm{D} = (\hbar v_s k_\mathrm{D})/k_B = 290\,\mathrm{K} \gg 20\,\mathrm{K}$, and this shows that the Debye approximation for the determination of the lattice specific heat of silver is reasonable at $T = 20\,\mathrm{K}$.

3. One has $c_v^\mathrm{ph} = (12\pi^4/5)nk_B(T/\Theta_\mathrm{D})^3 = 6.28\times10^4\,\mathrm{J/(K\cdot m^3)}$.

Exercise 2.

1. The bands are symmetric for $(k_x, k_y) \to (-k_x, k_y)$ and $(k_x, k_y) \to (k_x, -k_y)$, but not for $(k_x, k_y) \to (k_y, k_x)$, the spectrum is not invariant under a rotation by 60° around the $\Gamma = (0, 0)$ point, so the family to which the crystal belongs is orthorhombic.

2. The maximum of the valence band is found at the $\Gamma = (0, 0)$, point, where $E_{\rm v}(\Gamma) = \frac{7}{4}C = 0.7\,{\rm eV}$. The minimum of the conduction band is found at the $\Gamma = (0, 0)$, point, where $E_{\rm c}(\Gamma) = A - \frac{9}{5}B = 1.1\,{\rm eV}$. Therefore $E_g = E_{\rm c}(\Gamma) - E_{\rm v}(\Gamma) = 0.4\,{\rm eV}$. Since the two extrema are located at the same point of the Brillouin zone, the gap is direct.

3. The band dispersions along the ΓX and ΓS are shown in the left and right panel, respectively, of Fig. 2. Note the different scale along the energy axis.

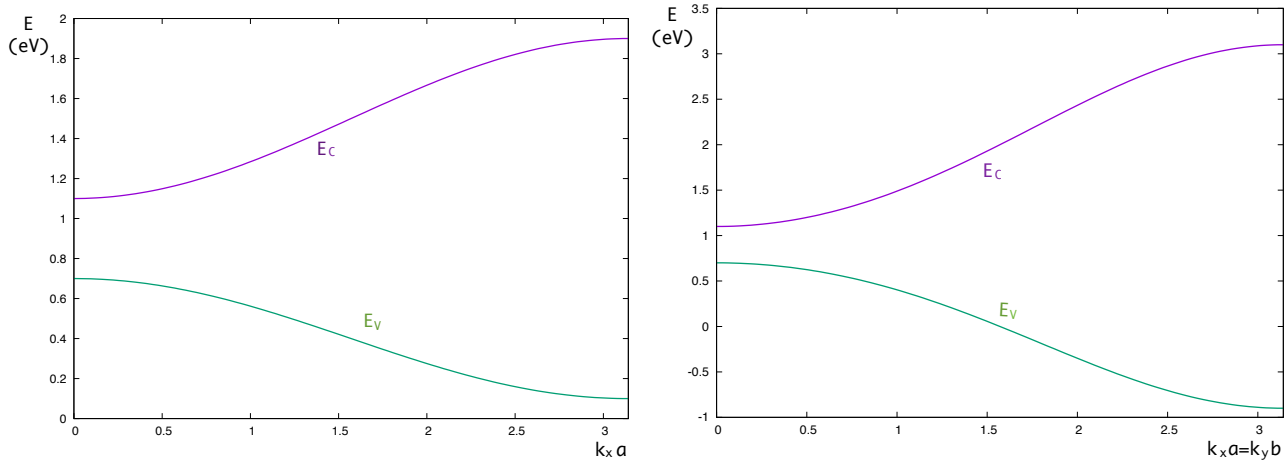

Fig. 2.

4. Expanding the expression of the conduction band around its minimum, one finds

$$E_{\rm c}(\boldsymbol{k}) \approx A - \frac{9}{5}B + \frac{\hbar^2}{2}\left(\frac{4}{5}\frac{B}{\hbar^2}\right)\left(a^2k_x^2 + b^2k_y^2\right).$$

Likewise, expanding the expression of the valence band around its maximum, one finds

$$E_{\rm v}(\boldsymbol{k}) \approx \frac{7}{4}C - \frac{\hbar^2}{2}\left(\frac{3}{4}\frac{C}{\hbar^2}\right)\left(a^2k_x^2 + b^2k_y^2\right).$$

Therefore, the mass tensor is diagonal in both bands, i.e., the principal axes of the mass tensor coincide with the high-symmetry axes of the orthorhombic structure. Reading the masses off the expressions of the dispersion laws, one finds $m^{\rm c}_{xy} = m^{\rm c}_{yx} = m^{\rm v}_{xy} = m^{\rm v}_{yx} = 0$, and

$$m^{\rm c}_{xx} = \frac{5\hbar^2}{4Ba^2} = 6.94\times10^{-31}\,{\rm kg} = 0.762\,m_0, \qquad m^{\rm c}_{yy} = \frac{5\hbar^2}{4Bb^2} = 1.08\times10^{-30}\,{\rm kg} = 1.19\,m_0,$$

$$m^{\rm v}_{xx} = \frac{4\hbar^2}{3Ca^2} = 9.26\times10^{-31}\,{\rm kg} = 1.02\,m_0, \qquad m^{\rm v}_{yy} = \frac{4\hbar^2}{3Cb^2} = 1.45\times10^{-30}\,{\rm kg} = 1.59\,m_0.$$