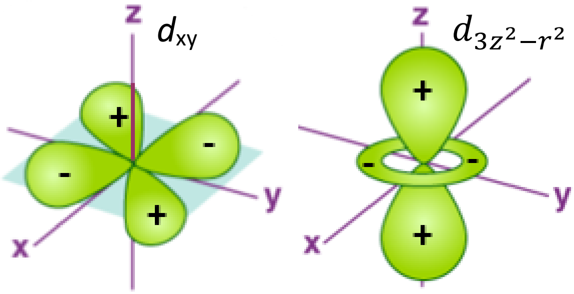
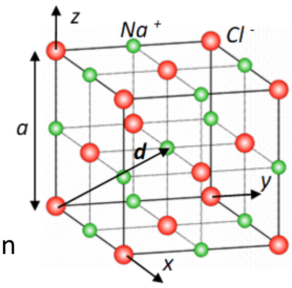
Condensed Matter Physics, written Exam of 17/07/2025 - Professors: M. Grilli and A. Polimeni

1) A two-dimensional crystal has a simple square lattice structure with unit cell a = 0.2 nm and two orbitals per unit cell: the d_{xy} with energy E_{xy} = -1.3 eV and the $d_{3z^2-r^2}$ with energy E_z = 1.0 eV. Knowing that the gap between the bands is E_g = 0.5 eV and that the hopping integral of the valence band is $|\gamma_{xy}|$=0.25 eV,

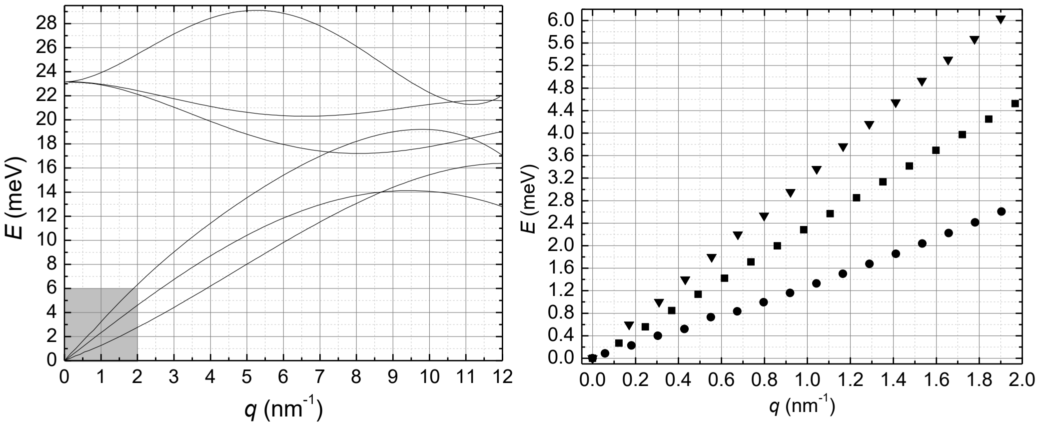


1) determine the hopping integral of the conduction band;
2) within the parabolic approximation determine the effective masses near the minimum of the conduction band and the maximum of the valence band and determine the density of states of the valence and conduction bands (remember that the lattice is 2D);
3) determine the number of carriers in the conduction band at T = 400 K assuming that the non-degeneracy condition is met (namely, $E_c-\mu >> k_BT$, where E_c is conduction band energy, μ is the chemical potential);
4) determine the conductivity at T = 400 K knowing that the mobility in the conduction and valence bands is μ_c = 2:0 $m^2/(V\cdot s)$ and μ_v = 1.5 $m^2/(V\cdot s)$, respectively.
Remember that $k_B = 1.3807 \times 10^{-23}$ J/K = 0.8617×10^{-4} eV/K and $\hbar = 1.05\times 10^{-34}$ J·s, 1 eV= 1.60219×10^{-19} J.

2) Sodium chloride (NaCl) is a face-centred cubic (fcc) lattice with a Na-Cl atom basis. The NaCl lattice can be regarded as two interpenetrating fcc primitive lattices displaced by $\boldsymbol{d}=a/2\,(x,y,z)$, where a is the side of the conventional unit cell (see figure on the right) and x,y,z are the Cartesian reference versors.



1) Determine the NaCl lattice constant knowing that the 7[th] diffraction peak in a powder x-ray experiment (λ = 0:15 nm) occurs at 70.848°.
2) The figures below show the phonon dispersion curves along the Γ-K direction of the first Brillouin zone (the figure on the right shows an enlarged portion of the entire dispersion curve, which is shown on the left). Determine the average sound velocity associated to that direction.



3) Determine the Debye temperature assuming the sound velocity determined above as the lattice average velocity.
4) Evaluate the specific heat at 10 K and 600 K.

[$\hbar=1.055\text{x}10^{-34}$ J·s; $k_B=1.381\text{x}10^{-23}$ J·K^{-1}]

Solution 1

1)

$$E_{xy}(k) = E_{xy} - 2\gamma_{xy}[\cos(ak_x) + \cos(ak_y)]$$

with $\gamma_{xy} < 0$

$$E_z - 2\gamma_z[\cos(ak_x) + \cos(ak_y)]$$

with $\gamma_z > 0$. Then the maximum of the valence band and the minimum of the conduction band both occur at $(0,0)$. Then $E_g = E_z - 4\gamma_z - E_{xy} + 4\gamma_{xy} = 0.5$. Therefore $\gamma_z = 0.2$ eV.

2)

$$m_{xy,z}^{-1} = \hbar^{-2}\frac{\partial^2 E_{xy,z}(k)}{\partial^2 k_x}$$

Thus $m_{xy} = \hbar^2/(2\gamma_{xy}a^2) = 0.36 \times 10^{-29} Kg = 3.9 m_e$ and $m_z = \hbar^2/(2\gamma_z a^2) = 4.9 m_e$. In two dimensions the DOS is given by

$$g(E) = \frac{1}{2\pi^2}\int d\mathbf{k}\delta(E - E(k)) = \frac{m}{\pi\hbar^2}.$$

3) Therefore

$$N_c(T) = \int_{E_c}^{\infty} dE g(E) e^{-(E-E_c)/K_B T} = \frac{m_z K_B T}{\pi\hbar^2}$$

and similarly for the holes in the valence band with $m_z \to m_{xy}$. Thus the number of intrinsic carriers is

$$n_i(T) = \sqrt{N_c(T)P_v(T)}e^{-E_g/2K_B T} = \frac{K_B T}{\pi\hbar^2}\sqrt{m_{xy}m_z}e^{-\frac{E_g}{2K_B T}} = 4.53 \times 10^{14}\, m^{-2}$$

4) The conductivity is:

$$\sigma(T = 400K) = qn_i(\mu_c + \mu_v) = 1.6 \times 10^{-19} \times 4.53 \times 10^{14} \times 3.50 = 2.54 \times 10^{-4}\,\Omega^{-1}.$$

Solution 2

1) Considering the fcc lattice structure of NaCl we have the following x-ray diffraction angles 2θ

1. Since

$$\theta = \arcsin\left(\frac{\lambda}{2d}\right) = \arcsin\left(\frac{\lambda}{a}\sqrt{h^2+k^2+l^2}\right),$$

where the indices h, k, l are all even or all odd, we find

	h	k	l	d (nm)	θ (deg)	2θ (deg)
1	1	1	1	0.32564	13.31578	26.63156
2	2	0	0	0.28201	15.42329	30.84658
3	2	2	0	0.19941	22.09277	44.18553
4	3	1	1	0.17006	26.16926	52.33858
5	2	2	2	0.16282	27.42812	54.85624
6	4	0	0	0.14142	32.13365	64.26730
7	3	3	1	0.12940	35.42384	70.84768
8	4	2	0	0.12612	36.48967	72.97934

with

Peak	$h^2+k^2+l^2$
1	3
2	4
3	8
4	11
5	12
6	16
7	19

The 7th peak corresponds to $a = \frac{\lambda}{2\sin(35.424°)}\sqrt{19}$=0.56402 nm.

2) and 3) Taking the ratio between the phonon energy and the wavevector in the linear region of the dispersion curves, one obtains:

q (nm-1)	E (meV)	v (m/s)	<v> (m/s)	θ_D (K)
1.5	2.00	2025.7 (t1)	2699	225
1.5	3.44	3484.2 (t2)		
1.5	4.81	4871.9 (l)		

where v=(E/q)/$\hbar$ and $< v >= \sqrt[3]{\frac{1}{\frac{1}{3}\left(\frac{1}{v_l^3}+\frac{1}{v_{t1}^3}+\frac{1}{v_{t2}^3}\right)}}$.

$$\theta_D = \frac{\hbar}{k_B}(6\pi^2 n)^{1/3} < v >$$

with n being the unit cell volume density equal to $4/(0.564 \times 10^{-9})^3 = 2.23 \times 10^{28}\ \mathrm{m}^{-3}$.

4) The low-T specific heat is given by the Debye model: $c_\mathrm{V} = 234 \left(\frac{T}{\theta_\mathrm{D}}\right)^3 n\mathrm{k_B} = 6.2 \times 10^3 \frac{\mathrm{J}}{\mathrm{K\,m^3}}$.

At T=600 K, we have $c_\mathrm{V} = 6n\mathrm{k_B} = 1.85 \times 10^6 \frac{\mathrm{J}}{\mathrm{K\,m^3}}$.