Written exam of Condensed Matter Physics - September 10th 2019
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Exercise 1: X ray scattering.

Sodium chloride (NaCl) crystallizes in a face-centered cubic lattice with a basis consisting of a sodium ion at $\mathbf{d}_1 = (0,0,0)$ and a chlorine ion at the center of the conventional cubic cell $\mathbf{d}_2 = (a/2)(1,1,1)$, with $a = 0.56402\,\mathrm{nm}$ (see Fig. 1, left panel).

1. Determine the first 8 angles, measured with respect to the incident beam direction (see Fig. 1, right panel), for which diffraction peaks are observed on a detector using the powder or Debye-Scherrer method. The x-ray beam wavelength is $\lambda = 0.15\,\mathrm{nm}$.

2. Say which peaks are more intense assuming that the atomic form factor f can be put equal to Z (i.e., the atomic number) times the amplitude of the wave scattered from one electron.

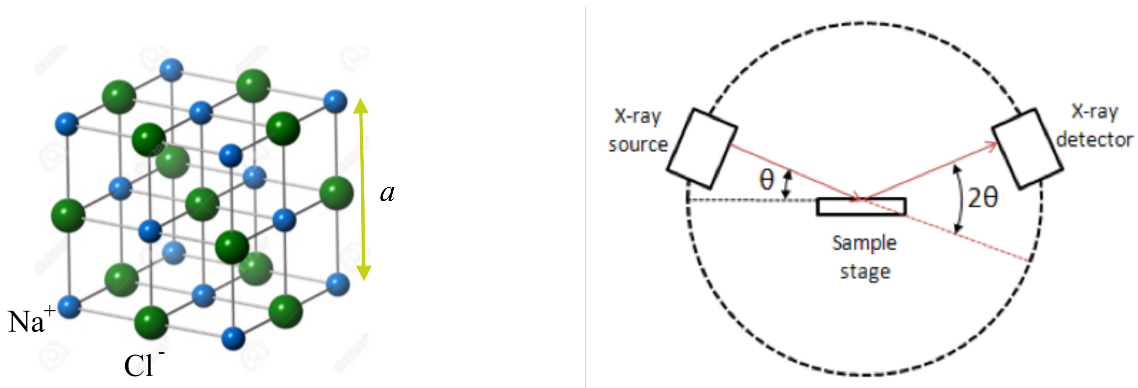

Fig. 1.

Exercise 2: Intrinsic semiconductors.

Consider a two-dimensional intrinsic semiconductor, that is described by the following density of states

$$D(\varepsilon) = \begin{cases} D_v, & \text{for } \varepsilon < \varepsilon_v, \\ D_c, & \text{for } \varepsilon > \varepsilon_c, \\ 0, & \text{elsewhere}, \end{cases}$$

such that the number of states per unit surface, in the interval $[\varepsilon, \varepsilon + \mathrm{d}\varepsilon]$, is $D(\varepsilon)\,\mathrm{d}\varepsilon$, with constant D_v and D_c, ε_v and ε_c being the thresholds of the valence and conduction band, respectively.

1. Determine the density of electrons in the conduction band, n, and the density of holes in the valence band, p, as a function of $D_v, D_c, \varepsilon_v, \varepsilon_c$, at a generic temperature T (assume, here and in the following, that the temperature is such that $\mu - \varepsilon_v, \varepsilon_c - \mu \gg \kappa_B T$, where μ is the chemical potential and κ_B is the Boltzmann constant).

2. Determine the expression of the chemical potential μ, as a function of $D_v, D_c, \varepsilon_v, \varepsilon_c$, at a generic temperature T.

3. Let now $D_v = 2.5 \times 10^{18}\,\mathrm{eV}^{-1}\cdot\mathrm{m}^{-2}$, $D_c = 5.0 \times 10^{18}\,\mathrm{eV}^{-1}\cdot\mathrm{m}^{-2}$, $\varepsilon_v = 1.05\,\mathrm{eV}$, $\varepsilon_c = 1.45\,\mathrm{eV}$, evaluate n, p and μ at $T = 300\,\mathrm{K}$.

[Note that $1\,\mathrm{eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,\mathrm{J}$; the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\mathrm{J}\cdot\mathrm{K}^{-1}$].

Solution of the written exam
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Exercise 1.

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

2. The resulting scattered amplitude is

$$\begin{aligned} I &= A\,\Big| f_{\rm Na}\left[\mathrm{e}^{-i0} + \mathrm{e}^{-i\pi(h+k)} + \mathrm{e}^{-i\pi(h+l)} + \mathrm{e}^{-i\pi(k+l)}\right] \\ &+\ f_{\rm Cl}\left[\mathrm{e}^{-i\pi(h+k+l)} + \mathrm{e}^{-i\pi(2h+2k+l)} + \mathrm{e}^{-i\pi(2h+k+2l)} + \mathrm{e}^{-i\pi(h+2k+2l)}\right]\Big|^2 \\ &= A\,\Big|\left[f_{\rm Na} + f_{\rm Cl}\,\mathrm{e}^{-i\pi(h+k+l)}\right]\left[1 + \mathrm{e}^{-i\pi(h+k)} + \mathrm{e}^{-i\pi(h+l)} + \mathrm{e}^{-i\pi(k+l)}\right]\Big|^2. \end{aligned}$$

The scattered amplitude is non zero provided the h, k, l indices are all even, and $I = 16\,A\,(f_{\rm Na} + f_{\rm Cl})^2$ (greater intensity), or all odd, and $I = 16\,A\,(f_{\rm Na} - f_{\rm Cl})^2$ (lower intensity).

Exercise 2.

1. We have

$$n = \int_{\varepsilon_c}^{+\infty} \frac{D_c}{\mathrm{e}^{(\varepsilon-\mu)/\kappa_B T} + 1}\,\mathrm{d}\varepsilon \approx D_c \int_{\varepsilon_c}^{+\infty} \mathrm{e}^{-(\varepsilon-\mu)/\kappa_B T}\,\mathrm{d}\varepsilon = \kappa_B T D_c\,\mathrm{e}^{-(\varepsilon_c-\mu)/\kappa_B T}, \tag{1}$$

and

$$p = \int_{-\infty}^{\varepsilon_v} D_v\left[1 - \frac{1}{\mathrm{e}^{(\varepsilon-\mu)/\kappa_B T} + 1}\right]\mathrm{d}\varepsilon \approx D_v \int_{-\infty}^{\varepsilon_v} \mathrm{e}^{(\varepsilon-\mu)/\kappa_B T}\,\mathrm{d}\varepsilon = \kappa_B T D_v\,\mathrm{e}^{(\varepsilon_v-\mu)/\kappa_B T}. \tag{2}$$

Multiplying Eq. (1) by Eq. (2), the dependence on μ drops and we find

$$np = (\kappa_B T)^2 D_c D_v\,\mathrm{e}^{(\varepsilon_v-\varepsilon_c)/\kappa_B T} \equiv n_i^2,$$

which is the *law of mass action* in the present situation. In an intrinsic semiconductor

$$n = p = n_i = \kappa_B T\sqrt{D_c D_v}\,\mathrm{e}^{(\varepsilon_v-\varepsilon_c)/2\kappa_B T}.$$

2. Dividing Eq. (1) by Eq. (2), and taking into account that $n = p$ in an intrinsic semiconductor, we find

$$1 = \frac{D_c}{D_v}\,\mathrm{e}^{(2\mu-\varepsilon_v-\varepsilon_c)/\kappa_B T} \qquad \Rightarrow \qquad 0 = \log\frac{D_c}{D_v} + \frac{2\mu-\varepsilon_v-\varepsilon_c}{\kappa_B T},$$

hence

$$\mu = \frac{1}{2}\left(\varepsilon_v + \varepsilon_c + \kappa_B T \log \frac{D_v}{D_c}\right).$$

3. At $T = 300\,\mathrm{K}$, we have $\kappa_B T = 0.0259\,\mathrm{eV}$, hence

$$p = n = n_i = 4.06 \times 10^{13}\,\mathrm{m}^{-2},$$

and

$$\mu = 1.24\,\mathrm{eV}.$$