Written exam of Condensed Matter Physics - January 26th 2021
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Exercise 1: X ray scattering and phonons [15 points].

$\alpha-$Sn (tin) crystallizes in the diamond structure. The density of $\alpha-$Sn is $\rho_{\alpha-\mathrm{Sn}} = 5.769 \times 10^3\,\mathrm{kg{\cdot}m^{-3}}$ and its atomic mass is $\mu_{\alpha-\mathrm{Sn}} = 118.7\,\mathrm{a.m.u.}$

1. Determine the atomic density ρ_{at} and the side a of the conventional cubic unit cell of $\alpha-$Sn [**4 points**].

2. The crystal structure of $\alpha-$Sn is investigated by means of X ray scattering within the Debye-Scherrer setup. The wavelength of the radiation is $\lambda = 0.125\,\mathrm{nm}$. Determine the scattering angles ϕ of the first 5 peaks that are compatible with the diamond selection rules, and the corresponding indices hkl of the cubic structure [**7 points**].

3. The velocity of sound of $\alpha-$Sn is $c_l = 3320\,\mathrm{m{\cdot}s^{-1}}$ in the longitudinal acoustic phonon branch and $c_t = 1610\,\mathrm{m{\cdot}s^{-1}}$ in the two transversal acoustic phonon branches. Determine the average sound velocity c_s (within the Debye approximation) and the Debye temperature Θ_{D} of the acoustic modes of $\alpha-$Sn [**4 points**].

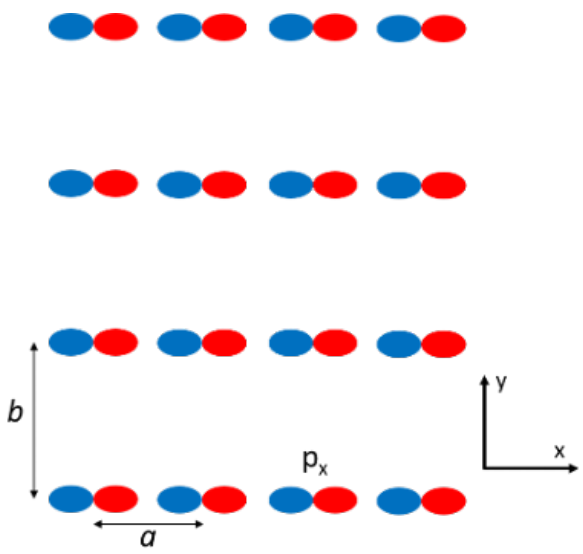

Fig. 1.

Exercise 2: Tight binding [15 points].

A two-dimensional rectangular crystal with lattice constants a and b (with $a < b$) hosts p_x-type orbitals (see Fig. 1). Assume that the electron states can be described within the tight binding model with attractive potential $\Delta U < 0$. Consider the interaction between the first neighbors only and let γ_x and γ_y be the transfer integral along the x and y directions.

1. Determine the sign of the transfer integrals and assign their absolute values knowing that γ can assume these two possible values: 1.0 eV and 2.0 eV [**2 points**].

2. Determine the energy vs. quasi-momentum dispersion relation $E(\boldsymbol{k})$, assuming that the overlap integrals are zero and that the energy of the atomic p_x level is $E_{px} = 3\,\mathrm{eV}$ [**4 points**].

3. Draw the first Brillouin zone and evaluate the band energy at the intersection points between the boundary of the first Brillouin zone and the reciprocal space axes, as well as at the zone centre [**4 points**].

4. Determine the expression of the effective mass tensor at the points specified above [**5 points**].

[Note that 1 a.m.u. corresponds to a mass of $1.661 \times 10^{-27}\,\mathrm{kg}$; 1 eV corresponds to an energy of $1.602 \times 10^{-19}\,\mathrm{J}$; the Planck constant is $\hbar = 1.055 \times 10^{-34}\,\mathrm{J{\cdot}s}$; the Boltzmann constant is $\kappa_B = 1.381 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$; the free electron mass is $m_0 = 9.109 \times 10^{-31}\,\mathrm{kg}$].

Solution of the written exam
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Exercise 1.

1. The atomic density of $\alpha-$Sn is

$$\rho_{\rm at} = \frac{\rho_{\alpha-{\rm Sn}}}{\mu_{\alpha-{\rm Sn}}} = 2.926 \times 10^{28}\,{\rm m}^{-3}.$$

Then, the lattice constant of the conventional cubic unit cell of $\alpha-$Sn is $a = (8/\rho_{\rm at})^{1/3} = 0.6490\,{\rm nm}$.

2. The first five peaks compatible with the diamond selection rules are those with Miller indices of the cubic structure equal to 111, 220, 311, 400, and 331. Then, by means of the Debye-Scherrer formula

$$\phi = 2\sin^{-1}\left(\frac{\lambda}{2d}\right), \qquad \text{with } d = \frac{a}{\sqrt{h^2+k^2+l^2}},$$

we find $\phi_1 = 19.20°$, $\phi_2 = 31.61°$, $\phi_3 = 37.25°$, $\phi_4 = 45.32°$, $\phi_5 = 49.64°$.

3. The average sound velocity in the Debye approximation is

$$c_s = \left[\frac{1}{3}\left(\frac{1}{c_l^3} + \frac{2}{c_t^3}\right)\right]^{-1/3} = 1809\,{\rm m\cdot s}^{-1}.$$

The Debye wave vector is $q_{\rm D} = (6\pi^2 n)^{1/3} = 9.534 \times 10^9\,{\rm m}^{-1}$, where $n = 4/a^3 = 1.463 \times 10^{28}\,{\rm m}^{-3}$ is the density of Bravais lattice points. The Debye temperature is

$$\Theta_{\rm D} = \frac{\hbar c_s q_{\rm D}}{\kappa_B} = 131.7\,{\rm K}.$$

Exercise 2.

1. We have

$$\gamma_x \equiv \gamma(a\hat{\boldsymbol{x}}) = -\int \mathrm{d}\boldsymbol{r}\, \varphi^*_{px}(\boldsymbol{r})\, \Delta U(\boldsymbol{r})\, \varphi_{px}(\boldsymbol{r} + a\hat{\boldsymbol{x}}) = -2\,\mathrm{eV} \equiv -t_x,$$
$$\gamma_y \equiv \gamma(b\hat{\boldsymbol{y}}) = -\int \mathrm{d}\boldsymbol{r}\, \varphi^*_{px}(\boldsymbol{r})\, \Delta U(\boldsymbol{r})\, \varphi_{px}(\boldsymbol{r} + b\hat{\boldsymbol{y}}) = 1\,\mathrm{eV} \equiv t_y.$$

2. The dispersion is

$$E(\boldsymbol{k}) = E_{px} - \sum_{\text{n.n.}} \gamma(\boldsymbol{R}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} = E_{px} + 2t_x \cos(a\, k_x) - 2t_y \cos(b\, k_y).$$

3. The Brillouin zone is shown in Fig. 2.

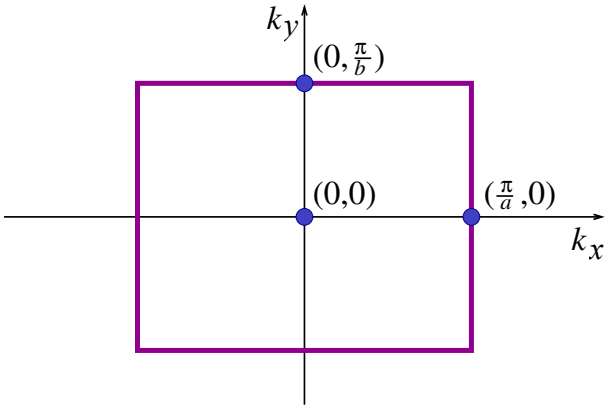

Fig. 2.

We have

$$E(0,0) = 5\,\mathrm{eV}; \qquad E\left(\frac{\pi}{a}, 0\right) = -3\,\mathrm{eV}; \qquad E\left(0, \frac{\pi}{b}\right) = 9\,\mathrm{eV};$$

4. The inverse mass tensor is

$$(m^*_{ij})^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 E(\boldsymbol{k})}{\partial k_i \partial k_j} = \frac{1}{\hbar^2}\begin{pmatrix} -2a^2 t_x \cos(a\, k_x) & 0 \\ 0 & 2b^2 t_y \cos(b\, k_y) \end{pmatrix}$$

Then:
• at $\boldsymbol{k} = (0,0)$

$$(m^*_{ij})^{-1} = \frac{1}{\hbar^2}\begin{pmatrix} -2a^2 t_x & 0 \\ 0 & 2b^2 t_y \end{pmatrix},$$

(this is a saddle point of the band dispersion);
• at $\boldsymbol{k} = \left(\frac{\pi}{a}, 0\right)$

$$(m^*_{ij})^{-1} = \frac{1}{\hbar^2}\begin{pmatrix} 2a^2 t_x & 0 \\ 0 & 2b^2 t_y \end{pmatrix},$$

(this is a minimum of the band dispersion);
• at $\boldsymbol{k} = \left(0, \frac{\pi}{b}\right)$

$$(m^*_{ij})^{-1} = \frac{1}{\hbar^2}\begin{pmatrix} -2a^2 t_x & 0 \\ 0 & -2b^2 t_y \end{pmatrix},$$

(this is maximum of the band dispersion).