Written exam of Condensed Matter Physics - November 4th 2022
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Exercise 1: Phonons.

Consider a one-dimensional monoatomic lattice having length $L = 40\,\text{cm}$. The phonon density of states, within the Debye model, is a constant $\mathcal{D} = 8.00 \times 10^{-5}\,\text{states/(rad/s)}$, for $0 \le \omega \le \omega_\text{D}$, where ω_D is the Debye frequency.

1. [4 points] Find the velocity of sound v_s of the given lattice.

2. [3 points] Evaluate the number of atoms N in the lattice, given the Debye frequency $\omega_\text{D} = 4.00 \times 10^{12}\,\text{rad/s}$.

3. [4 points] Determine the mass m of the atoms forming the lattice, knowing that the elastic constant that mimics the interaction between nearest-neighboring atoms is $\beta = 8.00 \times 10^{-3}\,\text{N/m}$.

3. [4 points] Evaluate the mean energy per unit length u at a temperature $T = 500\,\text{K}$, after checking that $\hbar\omega_\text{D} \ll \kappa_\text{B} T$, so that the classical approximation holds.

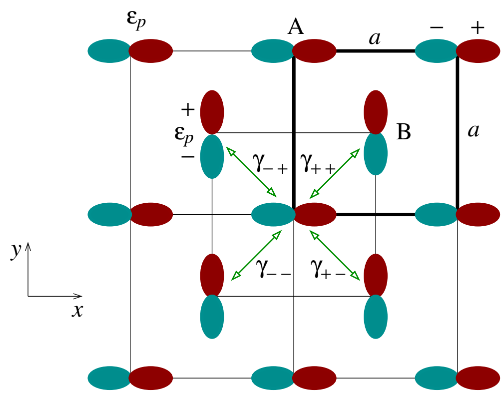

Fig. 1.

Exercise 2: Tight binding.

A binary compound AB forms a two-dimensional square Bravais lattice with lattice spacing $a = 0.5\,\text{nm}$ (see Fig. 1). The atoms A occupy the sites of the Bravais lattice, while the atoms B are located at the positions identified by the basis vector $\boldsymbol{d} = (a/2, a/2)$. A primitive cell is highlighted by a thicker line in Fig. 1. The atoms A display outer p_x orbitals, while the atoms B display outer p_y orbitals. The convention for the signs of the lobes of the p orbitals is shown in Fig. 1. The energy of both p orbitals is $\varepsilon_p = 0$. Assume that the electron states of the given lattice can be described within the tight-binding approximation with attractive lattice potential $\Delta U < 0$, and consider only nearest-neighbor transfer integrals $\gamma_{u\,v} \equiv \gamma\left(\boldsymbol{r}_{u\,v} \equiv u\frac{a}{2}\hat{\boldsymbol{x}} + v\frac{a}{2}\hat{\boldsymbol{y}}\right)$, where $u = \pm$, $v = \pm$, and $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ are the unit vectors of the corresponding axes, so that the four vectors $\boldsymbol{r}_{u\,v}$ locate the positions of the nearest neighbors. The absolute value of the nearest-neighbor transfer integrals is $\gamma_0 \equiv |\gamma_{u\,v}| = 0.75\,\text{eV}$. All other transfer integrals and all on-site (β) and overlap (α) integrals can be neglected.

1. [3 points] Assign the correct sign to the four nearest-neighbor transfer integrals, $\gamma_{+\,+}$, $\gamma_{+\,-}$, $\gamma_{-\,+}$, and $\gamma_{-\,-}$ (see Fig. 1), motivating your answer.

2. [5 points] Determine the two electron bands formed by the orbitals taken into account, $\varepsilon_\pm(\boldsymbol{k})$, where $\boldsymbol{k} = (k_x, k_y)$ is the two-dimensional Bloch wave vector.

3. [7 points] Determine the location of the minima of the lowest band $\varepsilon_-(\boldsymbol{k})$ in the first Brillouin zone, then calculate the numerical values of the eigenvalues of the effective mass tensor m_{ij}, $i = x, y$, $j = x, y$, at these points.

[Useful constants and conversion factors: the Planck constant is $\hbar = 1.05 \times 10^{-34}\,\text{J·s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,\text{J·K}^{-1}$, the elementary charge is $e = 1.60 \times 10^{-19}\,\text{C}$, the free electron mass is $m_0 = 9.11 \times 10^{-31}\,\text{kg}$; $1\,\text{eV}$ corresponds to a temperature of $1.16 \times 10^4\,\text{K}$ or to an energy of $1.60 \times 10^{-19}\,\text{J}$].

Solution
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Exercise 1.

1. One has

$$\mathcal{D}(\omega) = \frac{\mathrm{d}N}{\mathrm{d}\omega} = \frac{L}{\pi}\frac{\mathrm{d}q}{\mathrm{d}\omega} = \frac{L}{\pi v_s},$$

for $0 \le \omega \le \omega_{\mathrm{D}}$. Hence, one finds

$$v_s = \frac{L}{\pi \mathcal{D}} = 1.592 \times 10^3\,\mathrm{m/s}.$$

2. One has

$$N = \int_0^{\omega_{\mathrm{D}}} \mathcal{D}\,\mathrm{d}\omega = \mathcal{D}\,\omega_{\mathrm{D}} = 3.2 \times 10^8.$$

3. One has $v_s = a\sqrt{\beta/m}$, where $a = L/N$. Hence,

$$m = \left(\frac{L}{N}\right)^2 \frac{\beta}{v_s^2} = 4.93 \times 10^{-27}\,\mathrm{kg}.$$

4. One finds $\hbar\omega_{\mathrm{D}} = 4.22 \times 10^{-22}\,\mathrm{J} \ll \kappa_{\mathrm{B}}T = 6.90 \times 10^{-21}\,\mathrm{J}$, hence the classical approximation can be used and

$$u = \frac{\kappa_{\mathrm{B}}T}{a} = \frac{N\kappa_{\mathrm{B}}T}{L} = 5.52 \times 10^{-12}\mathrm{J/m}.$$

Exercise 2.

1. From Fig. 1 one can see that the positive lobe of the p_x orbital of an A atom is closer to the positive lobe of the p_y orbital a B atom at $\boldsymbol{r}_{+-}$ and to the negative lobe of the p_y orbital a B atom at $\boldsymbol{r}_{++}$, whereas the negative lobe of the p_x orbital of an A atom is closer to the negative lobe of the p_y orbital a B atom at $\boldsymbol{r}_{-+}$ and to the positive lobe of the p_y orbital a B atom at $\boldsymbol{r}_{--}$. Hence, for $\Delta U < 0$, $\gamma_{++} < 0$, $\gamma_{+-} > 0$, $\gamma_{-+} > 0$, and $\gamma_{--} < 0$.

2. Let

$$w_{\boldsymbol{k}} = \sum_{u=\pm}\sum_{v=\pm} \gamma_{u,v}\mathrm{e}^{\mathrm{i}\boldsymbol{r}_{u,v}\cdot\boldsymbol{k}} = 2\gamma_0\left\{\cos\left[\frac{a(k_x-k_y)}{2}\right] - \cos\left[\frac{a(k_x+k_y)}{2}\right]\right\} = 4\gamma_0 \sin\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y a}{2}\right).$$

Indicating with b_x and b_y the coefficients of the linear combination of p_x and p_y orbitals, respectively, within the tight-binding approximation indicated in the text, one find the text of two coupled homogeneous linear equations

$$\begin{cases} (\varepsilon_p - \varepsilon_{\boldsymbol{k}})b_x - w_{\boldsymbol{k}}\,b_y = 0, \\ -w_{\boldsymbol{k}}b_x + (\varepsilon_p - \varepsilon_{\boldsymbol{k}})b_x = 0, \end{cases}$$

which has nontrivial solutions if $\varepsilon_{\boldsymbol{k}} \equiv \varepsilon_\pm(\boldsymbol{k}) = \varepsilon_p \pm |w_{\boldsymbol{k}}|$. In the following, according to the text, we set $\varepsilon_p = 0$.

3. The minima of the lower band, $\varepsilon_-(\boldsymbol{k})$, are found where

$$\left|\sin\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y a}{2}\right)\right|$$

is maximum. In the first Brillouin zone $k_x \in [-\frac{\pi}{a}, \frac{\pi}{a}]$, $k_y \in [-\frac{\pi}{a}, \frac{\pi}{a}]$, this occurs at the four equivalent points $\boldsymbol{k}_{\pm\pm} = (\pm\frac{\pi}{a}, \pm\frac{\pi}{a})$, where the two sines are both equal to ± 1. Near the minima, then,

$$\varepsilon_-(\boldsymbol{k}) \approx -4\gamma_0 + \frac{1}{2}a^2\gamma_0\left(\delta k_x^2 + \delta k_y^2\right),$$

where δk_x and δk_y are the deviations of k_x and k_y with respect to their values at a given minimum. Hence, the inverse mass tensor is diagonal, and the two eigenvalues are equal, according to the symmetries of a square lattice. Thus, one finds

$$m_{xx} = m_{yy} = \frac{\hbar^2}{a^2\gamma_0} = 3.70 \times 10^{-31}\,\text{kg} = 0.406\,m_0.$$