Written exam of Condensed Matter Physics - November 14th 2019 (dedicated session)
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Exercise 1. Consider a one-dimensional crystal consisting of N units cells of size a (the total length of the crystal thus being $L = Na$), with a two-atom basis. All atoms are constrained to move only longitudinally. The two inequivalent atoms have masses $M = 4m$ and m, respectively, and are connected by inequivalent nearest-neighbor springs, whose elastic constant are $K_{\mathrm{S}} = 3K$ and $K_{\mathrm{L}} = K$, respectively [see Fig. 1(a)]. Indicate with u_n and v_n the displacement of atoms with mass M and m in the n-th unit cell, with respect to their equilibrium positions. Adopt Born-von Karman periodic boundary conditions. To assign numerical values, consider $a = 0.4\,\mathrm{nm}$, $m = 9.0 \times 10^{-26}\,\mathrm{kg}$, $K = 2.25\,\mathrm{kg/s^2}$.

1. Write the equations of motion for u_n and v_n. Then, assuming traveling-wave solutions $u_n = A\,\mathrm{e}^{i(qna-\omega t)}$ and $v_n = B\,\mathrm{e}^{i(qna-\omega t)}$, where q is the wave vector, determine the dispersion law of the acoustic and optical phonon branches, $\omega_a(q)$ and $\omega_o(q)$.

2. Find the dispersion law of the acoustic mode at small $|q|$, and determine the numerical value of the velocity of sound c_s.

3. Adopting a Debye model for the acoustic branch, $\omega_a(q) = c_s|q|$, and an Einstein model for the optical branch, with $\omega_E = \omega_o(q = 0)$, determine the low-temperature and high-temperature asymptotic expressions for the specific heat of the lattice (per unit length), c_L. Find the numerical value of c_L at $T = 3\,\mathrm{K}$, keeping in mind that $\int_0^\infty \frac{x}{\mathrm{e}^x-1}\,\mathrm{d}x = \frac{\pi^2}{6}$.

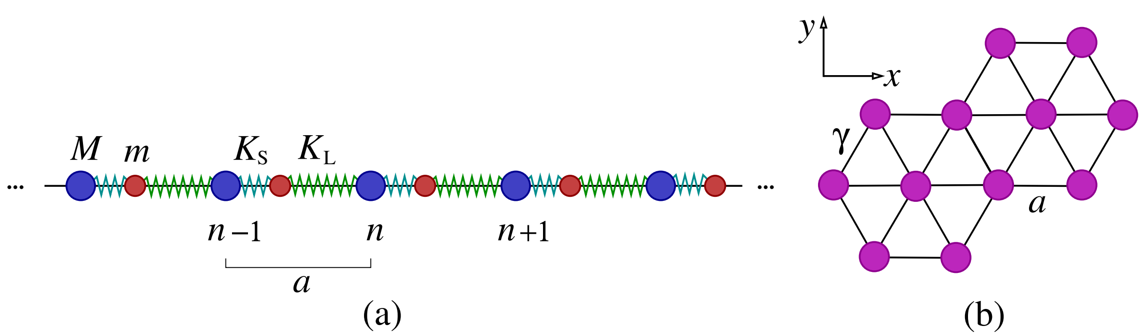

Fig. 1.

Exercise 2. Consider a two dimensional hexagonal Bravais lattice with lattice parameter $a = 0.5\,\mathrm{nm}$. The sites of the lattice are occupied by atoms with external s orbitals. The nearest-neighbor transfer integrals $\gamma = 0.15\,\mathrm{eV}$ are assigned [see Fig. 1(b)]. All other transfer integrals and all overlap integrals are negligible. The zero of the energy is set at the atomic level, $\varepsilon_s = 0$.

1. Determine the dispersion law $\varepsilon_{\boldsymbol{k}}$ of Bloch electrons on the given lattice within the tight-binding approximation, $\boldsymbol{k} = (k_x, k_y)$ being the wave vector.

2. Determine the expressions and the numerical values of the elements of the inverse effective mass tensor m_{ij}^{-1}, with $i, j = x, y$, at the Γ point of the Brillouin zone.

3. Determine the band width W.

[Useful constants and conversion factors: $k_B = 1.381 \times 10^{-23}\,\mathrm{J/K}$ (Boltzmann's constant), $\hbar = 1.055 \times 10^{-34}\,\mathrm{J{\cdot}s}$ (Planck's constant), $m_0 = 9.109 \times 10^{-31}\,\mathrm{kg}$ (electron mass); $1\,\mathrm{eV}$ corresponds to $1.602 \times 10^{-19}\,\mathrm{J}$].

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Exercise 1.

1. The equations of motion are

$$\begin{cases} M\,\ddot{u}_n = -K_{\rm S}\,(u_n - v_n) - K_{\rm L}\,(u_n - v_{n-1}) \\ m\,\ddot{v}_n = -K_{\rm S}\,(v_n - u_n) - K_{\rm L}\,(v_n - u_{n+1}) \end{cases} \quad \Rightarrow \quad \begin{cases} 4m\,\ddot{u}_n = -3K\,(u_n - v_n) - K\,(u_n - v_{n-1}) \\ m\,\ddot{v}_n = -3K\,(v_n - u_n) - K\,(v_n - u_{n+1})\,. \end{cases}$$

Substituting the traveling-wave solutions we find

$$\begin{cases} \left(4m\omega^2 - 4K\right)A + K\left(3 + {\rm e}^{-iqa}\right)B = 0 \\ K\left(3 + {\rm e}^{iqa}\right)A + \left(m\omega^2 - 4K\right)B = 0, \end{cases}$$

which admits nontrivial solutions for A, B if and only if the determinant of the matrix associated to the system of linear equations vanishes. Letting in the following $\overline{\Omega} \equiv \sqrt{K/m}$, which is the relevant frequency scale in our problem, the equation that determines the phonon frequencies is

$$\omega^4 - 5\,\overline{\Omega}^2\omega^2 + 3\,\overline{\Omega}^4 \sin^2\frac{qa}{2} = 0,$$

whose solutions are

$$\omega_\pm^2(q) = \frac{5}{2}\,\overline{\Omega}^2\left(1 \pm \sqrt{1 - \frac{12}{25}\sin^2\frac{qa}{2}}\right),$$

with $\omega_a(q) = \omega_-(q)$ and $\omega_o(q) = \omega_+(q)$ describing the acoustic and optical phonon branch, respectively.

2. For the acoustic branch, since for $|q|a \ll 1$ we have $\sin^2\frac{qa}{2} \approx \left(\frac{qa}{2}\right)^2$ and $\sqrt{1 - \frac{3}{25}(qa)^2} \approx 1 - \frac{3}{50}(qa)^2$, we find

$$\omega_a(q) \approx c_s|q|, \qquad \text{with } c_s = \frac{\sqrt{15}}{10}\,\overline{\Omega}a.$$

Inserting the values given in the text, $c_s = 774.6\,{\rm m/s}$.

3. We set $\omega_E \approx \omega_o(q=0) = \sqrt{5}\,\overline{\Omega} = 1.118 \times 10^{13}\,{\rm s}^{-1}$. Then, the internal energy per unit length is

$$u = \sum_{s=a,o}\int_{-\pi/a}^{\pi/a}\frac{{\rm d}q}{2\pi}\,\frac{\hbar\omega_s(q)}{{\rm e}^{\beta\hbar\omega_s(q)} - 1} \approx \int_0^{q_D}\frac{{\rm d}q}{\pi}\,\frac{\hbar c_s q}{{\rm e}^{\beta\hbar c_s q} - 1} + \frac{1}{a}\,\frac{\hbar\omega_E}{{\rm e}^{\beta\hbar\omega_E} - 1},$$

with $\beta = 1/(k_BT)$, and $q_D = \pi/a$, because in one dimension the Debye sphere coincides with the first Brillouin zone.

At high temperature, $k_BT \gg \hbar\omega_D, \hbar\omega_E$, with $\omega_D \equiv c_s q_D = \sqrt{15}\pi\overline{\Omega}/10 = 6.084 \times 10^{12}\,{\rm s}^{-1}$, the exponentials in the denominators can be expanded to first order, the two phonon modes give the same contribution (equipartition), and

$$u \approx \frac{2k_BT}{a} \quad \Rightarrow \quad c_L = \frac{2k_B}{a} \equiv c_L^{DP},$$

i.e., we recover the Dulong-Petit (DP) value for a one-dimensional crystal with two atoms per unit cell. For the given set of parameters $c_L \approx 6.903 \times 10^{-14}\,{\rm J/(K{\cdot}m)}$.

At low temperature, $k_BT \ll \hbar\omega_D, \hbar\omega_E$,

$$u \approx \frac{\hbar c_s}{\pi}\left(\frac{k_BT}{\hbar c_s}\right)^2\int_0^\infty\frac{x}{{\rm e}^x - 1}\,{\rm d}x + \frac{\hbar\omega_E}{a}{\rm e}^{-\beta\hbar\omega_E} \approx \frac{\pi^2\hbar\omega_D}{6a}\left(\frac{k_BT}{\hbar\omega_D}\right)^2 \quad \Rightarrow \quad c_L = \frac{\pi^2 k_B}{3a}\left(\frac{k_BT}{\hbar\omega_D}\right),$$

where we adopted the change of variable $x = \beta\hbar c_s q$ in the integral over q, and extended the integration limit to infinity, to extract the leading behavior at small T. In the final expression for u, we neglected the exponentially small contribution of the optical branch, since the numerical estimate gives $\Theta_E \equiv \hbar\omega_E/k_B = 85.39\,{\rm K}$, i.e., at $T = 3\,{\rm K}$, ${\rm e}^{-\beta\hbar\omega_E} \approx {\rm e}^{-28.46} \approx 4.3 \times 10^{-13}$. Thus, at $T = 3\,{\rm K}$, $c_L \approx 0.2124\,k_B/a = 0.0162\,c_L^{DP} = 7.327 \times 10^{-15}\,{\rm J/(K{\cdot}m)}$, where we used the numerical value of the Debye temperature $\Theta_D \equiv \hbar\omega_D/k_B = 46.47\,{\rm K}$.

Exercise 2.

1. The tight-binding dispersion law is

$$\varepsilon_{\boldsymbol{k}} = -\gamma \sum_{\boldsymbol{R}=\mathrm{nn}} \mathrm{e}^{i\boldsymbol{R}\cdot\boldsymbol{k}},$$

where the sum over $\boldsymbol{R}$ runs on the six nearest-neighbor lattice vectors $(0, \pm a)$, $\pm\frac{a}{2}(1, \sqrt{3})$, $\pm\frac{a}{2}(1, -\sqrt{3})$. Hence,

$$\varepsilon_{\boldsymbol{k}} = -2\gamma \left[\cos(ak_x) + 2\cos\left(\frac{1}{2}ak_x\right)\cos\left(\frac{\sqrt{3}}{2}ak_y\right)\right].$$

2. Expanding $\varepsilon_{\boldsymbol{k}}$ near the Γ point, we find

$$\varepsilon_{\boldsymbol{k}} \approx -6\gamma + \frac{3}{2}a^2\gamma\left(k_x^2 + k_y^2\right),$$

whence it is evident that

$$m_{xx}^{-1} = m_{yy}^{-1} = \frac{3a^2\gamma}{\hbar^2} = 1.621 \times 10^{30}\,\mathrm{kg}^{-1} = 1.456\,m_0^{-1}, \qquad m_{xy}^{-1} = m_{yx}^{-1} = 0.$$

3. Taking the derivatives

$$\frac{\partial\varepsilon_{\boldsymbol{k}}}{\partial k_x} = 2\gamma a \sin\left(\frac{1}{2}ak_x\right)\left[2\cos\left(\frac{1}{2}ak_x\right) + \cos\left(\frac{\sqrt{3}}{2}ak_y\right)\right], \qquad \frac{\partial\varepsilon_{\boldsymbol{k}}}{\partial k_y} = 2\sqrt{3}\gamma a \cos\left(\frac{1}{2}ak_x\right)\sin\left(\frac{\sqrt{3}}{2}ak_y\right),$$

we find that the extrema of the band dispersion are located where

$$\begin{cases} \sin\left(\frac{1}{2}ak_x\right) = 0, \\ \sin\left(\frac{\sqrt{3}}{2}ak_y\right) = 0, \end{cases} \quad \text{or} \quad \begin{cases} \cos\left(\frac{1}{2}ak_x\right) = 0, \\ \cos\left(\frac{\sqrt{3}}{2}ak_y\right) = 0, \end{cases} \quad \text{or} \quad \begin{cases} \cos\left(\frac{1}{2}ak_x\right) = \pm\frac{1}{2}, \\ \sin\left(\frac{\sqrt{3}}{2}ak_y\right) = 0. \end{cases}$$

Calculating the band dispersion in the various points, we find that the minimum is at Γ, where $\varepsilon_{\boldsymbol{k}} = -6\gamma$, whereas the maxima are found at $k_x = \frac{4\pi}{3a}$, $k_y = 0$, and all the equivalent points, where $\varepsilon_{\boldsymbol{k}} = 3\gamma$, hence the band width is $W = 9\gamma = 1.35\,\mathrm{eV}$.