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Condensed Matter Theory 1 — Exercise 4

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`https://ilias.studium.kit.edu/goto.php?target=crs_2219528`
To be discussed on: *Thursday 2023/11/23*

1. Phonons of the two-dimensional triangular lattice

Consider a triangular Bravais lattice $\vec{R}^{(0)}_{j,l} = j\vec{a}_1 + l\vec{a}_2$ with $j, l \in \mathbb{Z}$, see Fig. 1(a), and lattice constant $a = |\vec{a}_1| = |\vec{a}_2|$. At equilibrium, point particles with mass M are located at each lattice point. Each particle is interacting with its nearest neighbours via springs with spring constant γ.

In the following, we consider small-amplitude oscillations of the particles around their equilibrium positions $\vec{R}^{(0)}_{j,l}$. They are described by the position vectors $\vec{R}_{j,l}(t) = \vec{R}^{(0)}_{j,l} + \vec{u}\left(\vec{R}^{(0)}_{j,l}, t\right)$, where the magnitude of deviations $|\vec{u}| \ll a$ is small compared to the lattice constant a. The Hamiltonian of the system reads

$$\mathcal{H} = \sum_{j,l} \left[\frac{\vec{P}^2_{j,l}}{2M} + V_{j,l}(\{\vec{R}_{n,m}\}) \right], \tag{1}$$

where $\vec{P}_{j,l}$ is the momentum of the mass with equilibrium position $\vec{R}^{(0)}_{j,l}$.

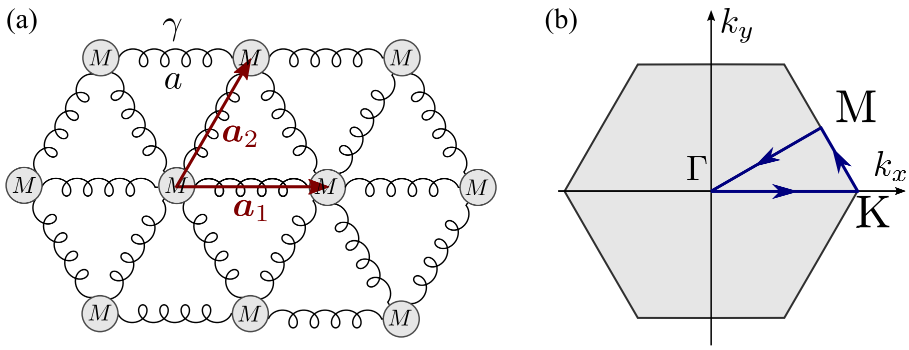

Figure 1: (a) Triangular Bravais lattice and (b) its first Brillouin zone

a) Show that in the harmonic approximation the potential can be written in the form

$$V_{j,l} = \frac{\gamma}{2}\frac{1}{a^2} \sum_{\vec{\delta}_i} \left(\vec{\delta}_i \cdot \left[\vec{u}\left(\vec{R}^{(0)}_{j,l}\right) - \vec{u}\left(\vec{R}^{(0)}_{j,l} + \vec{\delta}_i\right) \right] \right)^2,$$

where the summation is over the three nearest-neighbor vectors $\vec{\delta}_1 = a(1,0)^T, \vec{\delta}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)^T$ and $\vec{\delta}_3 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)^T$

b) Use the transformations

$$\vec{u}\left(\vec{R}^{(0)}_{j,l}\right) = \frac{\sqrt{V_{\mathrm{PUC}}}}{\sqrt{M}} \int\limits_{1.\mathrm{BZ}} \frac{\mathrm{d}\vec{k}}{(2\pi)^2} e^{i\vec{k}\cdot\vec{R}^{(0)}_{j,l}} \vec{q}(\vec{k}), \qquad \vec{P}_{j,l} = \sqrt{V_{\mathrm{PUC}}}\sqrt{M} \int\limits_{1.\mathrm{BZ}} \frac{\mathrm{d}\vec{k}}{(2\pi)^2} e^{-i\vec{k}\cdot\vec{R}^{(0)}_{j,l}} \vec{p}(\vec{k}) \tag{2}$$

to cast the Hamiltonian (1) into the form

$$\mathcal{H} = \int\limits_{1.\mathrm{BZ}} \frac{\mathrm{d}\vec{k}}{(2\pi)^2} \frac{1}{2} \left[\vec{p}(\vec{k})\cdot\vec{p}(-\vec{k}) + \vec{q}(\vec{k})\cdot\mathbf{D}(\vec{k})\cdot\vec{q}(-\vec{k})\right] . \tag{3}$$

Here, $\mathbf{D}$ is the dynamical matrix given by

$$\mathbf{D}(\vec{k}) = \frac{2\gamma}{M}\begin{pmatrix} \eta_0+\eta_3 & \eta_1 \\ \eta_1 & \eta_0-\eta_3 \end{pmatrix}, \tag{4}$$

with $A_i = \sin^2\left(\frac{\vec{k}\cdot\vec{\delta}_i}{2}\right)$, $\eta_0 = \sum_i A_i$, $\eta_1 = \frac{\sqrt{3}}{2}(A_2 - A_3)$, and $\eta_3 = A_1 - \frac{1}{2}(A_2 + A_3)$.

c) Let d_n be the eigenvalues of the dynamical matrix $\mathbf{D}$ with $n = 1, 2$. Show that the phonon eigenenergy $\omega_n = \sqrt{d_n}$ is

$$d_{1,2} = \frac{2\gamma}{M}\left(\eta_0 \pm \sqrt{\eta_1^2+\eta_3^2}\right) \tag{5}$$

$$\omega_{1,2} = \sqrt{\frac{2\gamma}{M}}\left[A_1 + A_2 + A_3 \pm \sqrt{A_1^2 + A_2^2 + A_3^2 - A_1A_2 - A_2A_3 - A_3A_1}\right]^{1/2} . \tag{6}$$

d) Plot the obtained dispersion relations $\omega_n(\vec{k})$ along the path $\Gamma KM\Gamma$ shown in Fig. 1(b).

e) For the case $|\vec{k}|a \ll 1$, determine the sound velocities for both branches. How do these velocities depend on the direction of the wavevector $\vec{k}$?

f) Along the path ΓK, analyze the polarization vectors $\vec{\varepsilon}_n$, where $\mathbf{D}\cdot\vec{\varepsilon}_n = d_n\vec{\varepsilon}_n$. Determine which of the branches is longitudinal, i.e., $\vec{\varepsilon}_n || \vec{k}$ and which one is transversal $\vec{\varepsilon}_n \perp \vec{k}$.

2. Absence of long-range crystalline order in 1d

Consider a one-dimensional chain of atoms with mass m. The Hamiltonian of their phonon excitations reads

$$\mathcal{H} = \sum_{k\in 1.\mathrm{BZ}} \hbar\omega_k (a_k^\dagger a_k + \frac{1}{2}) \tag{6}$$

where a is the lattice spacing, L is the length of the sample, and $a_k^\dagger$ and a_k are creation and annihilation operators. The phonon dispersion is $\omega_k = \omega_{-k}$. The deviation of the atom at site x_i from its equilibrium position is given by

$$u_i = \frac{1}{\sqrt{N}} \sum_{k\in 1.\mathrm{BZ}} \sqrt{\frac{\hbar}{2m\omega_k}} (a_{-k} + a_k^\dagger) e^{ikx_i} \tag{7}$$

a) Determine the thermal expectation value $\mathcal{S}(x_i - x_j) = \langle u_i u_j \rangle$. Show that it takes the form

$$\mathcal{S}(x) = \frac{1}{N} \sum_{k \in 1.\mathrm{BZ}} \frac{\hbar}{2m\omega_k} \cos(kx)(1 + 2n_B(\hbar\omega_k)) \tag{8}$$

with the Bose function $n_B(\varepsilon) = 1/(\exp(\frac{\varepsilon}{k_B T}) - 1)$.

b) Show that $\mathcal{S}(0)$ diverges at temperature $T = 0$ as well as $T > 0$. This quantity appears in the exponent of the Debye-Waller factor. Why does the diverging result imply the absence of long-range crystalline order?
Hint: To extract the divergent behavior, replace the sum $\frac{1}{N}\sum_{k\in 1.\mathrm{BZ}}$ by an integral $a\int \frac{dk}{2\pi}$. It is sufficient to integrate only over the range of small momenta $a\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi}$, where Λ is a momentum cutoff, for which the phonon dispersion can be approximated to be linear $\omega(k) \approx c|k|$ with the sound velocity c.