Karlsruhe Institute of Technology — Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I   WS 2022/2023

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Sheet 11
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Category A

1. Phonons in two-dimensional triangular lattice (15+10=25 Points)

Consider a two-dimensional triangular lattice of particles of mass m and lattice constant a. Let $\vec{r}_{i,j}$ is a set of six unit vectors pointing from the equilibrium location $\vec{R}_i$ of the particle i to the equilibrium location of six nearest neighbor particles with the coordinates $\vec{R}_j$. Let $\vec{u}_i$ gives the two-dimensional displacement of the particle i from its equilibrium location. Suppose that the force acting on the particle i is $\vec{F}_i = m\omega_0^2 \sum_j \vec{r}_{i,j}\big(\vec{r}_{i,j}\cdot(\vec{u}_j - \vec{u}_i)\big)$. (Note that j in the sum indexes the six nearest neighbors of i.)

(a) Consider the Newtonian equation of motion of i-particle, $m\dfrac{d^2\vec{u}_i}{dt^2} = \vec{F}_i$, where the displacement at the moment of time t is $u_i(t)$. Use the plane wave ansatz of the form $\vec{u}_{j,\vec{k}}(t) = A_{\vec{k}} e^{i\vec{R}_j\vec{k} - i\omega_{\vec{k}}t}$, derive a set of two equations on the components of the vector $\vec{A} = \begin{pmatrix} A_x \\ A_y \end{pmatrix}$, which determines the amplitude of the plane wave of the momentum $\vec{k}$ and frequency $\omega_{\vec{k}}$. Obtain the equation for the dispersion relation $\omega_{\vec{k}}$ for vibrations of the lattice.

Solution: The unit vectors for all j read $\mathbf{r}_{1,j} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\mathbf{r}_{2,j} = \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix}$, $\mathbf{r}_{3,j} = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix}$, $\mathbf{r}_{4,j} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$, $\mathbf{r}_{5,j} = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix}$, $\mathbf{r}_{6,j} = \begin{pmatrix} 1/2 \\ -\sqrt{3}/2 \end{pmatrix}$. The force $\vec{F}_i$ can be written in a matrix form:

$$\mathbf{F}_i = m\omega_0^2 \sum_j \mathbf{r}_{i,j}\mathbf{r}_{i,j}^T(\mathbf{u}_j - \mathbf{u}_i) = 2m\omega_0 e^{i\mathbf{k}\mathbf{R}_i - i\omega_{\mathbf{k}}t}\left(\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}(\cos(ak_x) - 1) + \right.$$

$$\left. + \begin{bmatrix} 1/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & 3/4 \end{bmatrix}(\cos a\frac{k_x + \sqrt{3}k_y}{2} - 1) + \begin{bmatrix} 1/4 & -\sqrt{3}/4 \\ -\sqrt{3}/4 & 3/4 \end{bmatrix}(\cos a\frac{k_x - \sqrt{3}k_y}{2} - 1)\right)\begin{bmatrix} A_x \\ A_y \end{bmatrix} =$$

$$= -m\omega_0^2 e^{i\mathbf{k}\mathbf{R}_i - i\omega_{\mathbf{k}}t} M_{\mathbf{k}} \begin{bmatrix} A_x \\ A_y \end{bmatrix},$$

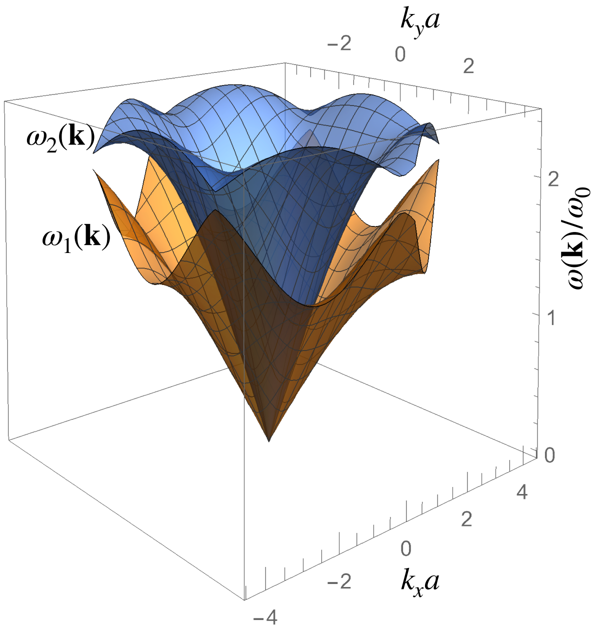
$$\text{where } M_{\mathbf{k}} = \begin{bmatrix} 3 - 2\cos(ak_x) - \cos\frac{ak_x}{2}\cos\frac{a\sqrt{3}k_y}{2} & \sqrt{3}\sin\frac{ak_x}{2}\sin\frac{a\sqrt{3}k_y}{2} \\ \sqrt{3}\sin\frac{ak_x}{2}\sin\frac{a\sqrt{3}k_y}{2} & 3 - 3\cos\frac{ak_x}{2}\cos\frac{a\sqrt{3}k_y}{2} \end{bmatrix}$$

The classical equation of motion becomes $\omega_{\mathbf{k}}^2 \begin{bmatrix} A_x \\ A_y \end{bmatrix} = \omega_0^2 M_{\mathbf{k}} \begin{bmatrix} A_x \\ A_y \end{bmatrix}$. This yields the eigenvalue problem: $\det(\omega_{\mathbf{k}}^2 - \omega_0^2 M_{\mathbf{k}}) = 0$. This equation has two solutions,

$$\omega_{1,2}(\mathbf{k}) = \Bigg(3 - 2\cos ak_x - \cos\frac{ak_x}{2}\cos\frac{a\sqrt{3}k_y}{2} \mp$$

$$\mp\frac{1}{\sqrt{2}}\sqrt{3 - 4\cos\frac{ak_x}{2}\cos ak_x\cos\frac{\sqrt{3}ak_y}{2} + (2\cos(ak_x) - 1)\cos\sqrt{3}ak_y - \cos ak_x + \cos 2ak_x}\Bigg)^{\frac{1}{2}},$$

that determine two phonon modes (see Figure).



(b) Take the long wavelength limit, i.e., $k \to 0$, and find the transverse and longitudinal phonon velocities of the lattice. (The transverse component of the velocity is perpendicular to $\vec{k}$ and the longitudinal one is parallel to $\vec{k}$.)

Solution: In the long wavelength limit, $k_{x,y} \ll \frac{1}{a}$, the matrix $M_{\mathbf{k}}$ in the leading order in $\mathbf{k}$ reads

$$M_{\mathbf{k}\to 0} \approx \begin{pmatrix} \frac{3a^2}{8}\left(3k_x^2 + k_y^2\right) & \frac{a^2}{4}(3k_xk_y) \\ \frac{a^2}{4}(3k_xk_y) & \frac{3a^2}{8}\left(k_x^2 + 3k_y^2\right) \end{pmatrix}.$$

The solution of $\det(\omega_{\mathbf{k}}^2 - \omega_0^2 M_{\mathbf{k}\to 0}) = 0$ and the respective eigenvectors read:

$$\omega_1(\mathbf{k}\ll a^{-1}) = \frac{\sqrt{3}}{2\sqrt{2}}a\omega_0|\mathbf{k}|, \quad \vec{A}_1 \sim \begin{bmatrix} k_x \\ -k_y \end{bmatrix},$$

and

$$\omega_2(\mathbf{k}\ll a^{-1}) = \frac{3}{2\sqrt{2}}a\omega_0|\mathbf{k}|, \quad \vec{A}_2 \sim \begin{bmatrix} k_x \\ k_y \end{bmatrix}.$$

The eigenvector $\vec{A}_1$ is perpendicular to $\mathbf{k}$, i.e., the mode ω_1 is transversal; it has the velocity $v_1 = \frac{\sqrt{3}}{2\sqrt{2}}a\omega_0$. The eigenvector $\vec{A}_2$ is parallel to $\mathbf{k}$, i.e., the mode ω_2 is longitudinal and has the velocity $v_2 = \frac{3}{2\sqrt{2}}a\omega_0$.

Category B

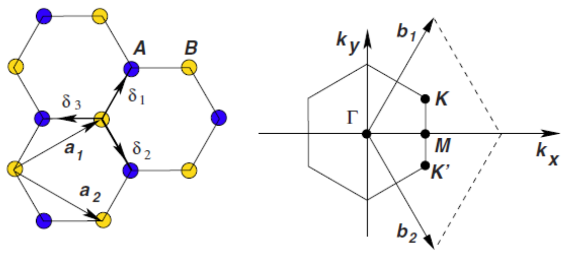
2. Phonons in graphene (25 Points)

Consider the honeycomb lattice in graphene. Let $\mathbf{R}^{(\mathbf{A})}_{\mathbf{m,n}}$ and $\mathbf{R}^{(\mathbf{B})}_{\mathbf{m,n}}$ denotes respectively the position of ions in sublattice A and B where m and n stand for the indices of the Bravais cell. The distance between neighbouring ions A and B at rest is set to 1 and one considers only nearest-neighbor couplings within harmonic approximation. The potential energy between neighbouring ions is given by:

$$U = \frac{K}{2}\sum_{m,n}\left[\left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m,n}\right| - 1\right)^2 + \left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m,n-1}\right| - 1\right)^2 + \left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m-1,n}\right| - 1\right)^2\right].$$

Find the phonon spectrum of graphene assuming that the carbon atoms move only within the two-dimensional plane.

Solution:



The position of each ion can be represented by the average position $\boldsymbol{R}^{(0)}$ (position at rest) plus a deviation $\boldsymbol{u}$ (displacement field). There are two ions (A and B) per unit cell.

$$\boldsymbol{R}^{A(0)}_{m,n} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2,$$

and

$$\boldsymbol{R}^{B(0)}_{m,n} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2 - \boldsymbol{\delta}_3,$$

where the lattice vectors are:

$$\boldsymbol{a}_1 = \boldsymbol{\delta}_1 - \boldsymbol{\delta}_3 = \frac{\sqrt{3}}{2}\left(\sqrt{3}, 1\right), \quad \boldsymbol{a}_2 = \boldsymbol{\delta}_2 - \boldsymbol{\delta}_3 = \frac{\sqrt{3}}{2}\left(\sqrt{3}, -1\right),$$

where $\boldsymbol{\delta}_j$ points to the nearest neighbor (see Figure):

$$\boldsymbol{\delta}_1 = \frac{1}{2}\left(1, \sqrt{3}\right), \quad \boldsymbol{\delta}_2 = \frac{1}{2}\left(1, -\sqrt{3}\right), \quad \boldsymbol{\delta}_3 = (-1, 0).$$

Now, the position of ions A and B can be written as:

$$\boldsymbol{R}^{(A)}_{m,n} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2 + \boldsymbol{u}^{(A)}_{m,n}, \quad \boldsymbol{R}^{(B)}_{m,n} = m\boldsymbol{a}_1 + n\boldsymbol{a}_2 - \boldsymbol{\delta}_3 + \boldsymbol{u}^{(B)}_{m,n}.$$

The potential energy is:

$$U = \frac{K}{2}\sum_{m,n}\left[\left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m,n}\right| - 1\right)^2 + \left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m,n-1}\right| - 1\right)^2 + \left(\left|\boldsymbol{R}^{(A)}_{m,n} - \boldsymbol{R}^{(B)}_{m-1,n}\right| - 1\right)^2\right].$$

When we develop the expression up to order 2 we obtain in $\boldsymbol{u}$:

$$U_{m,n}^{(A)} = \frac{K}{2}\left\{\left[\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x - \left(\boldsymbol{u}_{m,n}^{(B)}\right)_x\right]^2 \right.$$
$$+\frac{1}{4}\left[\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x - \left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_x - \sqrt{3}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_y + \sqrt{3}\left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_y\right]^2$$
$$\left.+\frac{1}{4}\left[\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x - \left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_x + \sqrt{3}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_y - \sqrt{3}\left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_y\right]^2\right\}.$$

Equation of motions are:

$$M\frac{d^2}{dt^2}\left(\boldsymbol{u}_{m,n}^{(A,B)}\right)_{x,y} = -\frac{\partial U}{\partial\left(\boldsymbol{u}_{m,n}^{(A,B)}\right)_{x,y}}.$$

Explicitely it gives:

$$-\frac{M}{K}\frac{d^2}{dt^2}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x = \frac{3}{2}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x - \left[\left(\boldsymbol{u}_{m,n}^{(B)}\right)_x + \frac{1}{4}\left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_x + \frac{1}{4}\left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_x\right]$$
$$+\frac{\sqrt{3}}{4}\left[\left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_y - \left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_y\right],$$

$$-\frac{M}{K}\frac{d^2}{dt^2}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_y = \frac{3}{2}\left(\boldsymbol{u}_{m,n}^{(A)}\right)_y - \frac{3}{4}\left[\left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_y + \left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_y\right]$$
$$+\frac{\sqrt{3}}{4}\left[\left(\boldsymbol{u}_{m,n-1}^{(B)}\right)_x - \left(\boldsymbol{u}_{m-1,n}^{(B)}\right)_x\right],$$

$$-\frac{M}{K}\frac{d^2}{dt^2}\left(\boldsymbol{u}_{m,n}^{(B)}\right)_x = \frac{3}{2}\left(\boldsymbol{u}_{m,n}^{(B)}\right)_x - \left[\left(\boldsymbol{u}_{m,n}^{(A)}\right)_x + \frac{1}{4}\left(\boldsymbol{u}_{m,n+1}^{(A)}\right)_x + \frac{1}{4}\left(\boldsymbol{u}_{m+1,n}^{(A)}\right)_x\right]$$
$$+\frac{\sqrt{3}}{4}\left[\left(\boldsymbol{u}_{m,n+1}^{(A)}\right)_y - \left(\boldsymbol{u}_{m+1,n}^{(A)}\right)_y\right],$$

$$-\frac{M}{K}\frac{d^2}{dt^2}\left(\boldsymbol{u}_{m,n}^{(B)}\right)_y = \frac{3}{2}\left(\boldsymbol{u}_{m,n}^{(B)}\right)_y - \frac{3}{4}\left[\left(\boldsymbol{u}_{m,n+1}^{(A)}\right)_y + \left(\boldsymbol{u}_{m+1,n}^{(A)}\right)_y\right]$$
$$+\frac{\sqrt{3}}{4}\left[\left(\boldsymbol{u}_{m,n+1}^{(A)}\right)_x - \left(\boldsymbol{u}_{m+1,n}^{(A)}\right)_x\right].$$

Using the Fourier transform of $\mathbf{u}$:

$$\left(\boldsymbol{u}_{m,n}^{(A,B)}\right)_{x,y} = A_{x,y}^{(A,B)} e^{i\omega t} e^{-i\boldsymbol{R}_{m,n}^{A(0)}\cdot\boldsymbol{q}},$$

The dispersion relation is written in matrix form:

$$\frac{M}{K}\,\omega^2\boldsymbol{A} = \frac{1}{4}\widehat{\mathcal{D}}\boldsymbol{A},$$

where

$$\boldsymbol{A}^T = \left(A_x^{(A)}, A_y^{(A)}, A_x^{(B)}, A_y^{(B)}\right),$$

and

$$\widehat{\mathcal{D}} = \begin{pmatrix} 6 & 0 & -\left[4 + e^{i\boldsymbol{a}_2\boldsymbol{q}} + e^{i\boldsymbol{a}_1\boldsymbol{q}}\right] & \sqrt{3}\left[e^{i\boldsymbol{a}_2\boldsymbol{q}} - e^{i\boldsymbol{a}_1\boldsymbol{q}}\right] \\ 0 & 6 & \sqrt{3}\left[e^{i\boldsymbol{a}_2\boldsymbol{q}} - e^{i\boldsymbol{a}_1\boldsymbol{q}}\right] & -3\left[e^{i\boldsymbol{a}_2\boldsymbol{q}} + e^{i\boldsymbol{a}_1\boldsymbol{q}}\right] \\ -\left[4 + e^{-i\boldsymbol{a}_2\boldsymbol{q}} + e^{-i\boldsymbol{a}_1\boldsymbol{q}}\right] & \sqrt{3}\left[e^{-i\boldsymbol{a}_2\boldsymbol{q}} - e^{-i\boldsymbol{a}_1\boldsymbol{q}}\right] & 6 & 0 \\ \sqrt{3}\left[e^{-i\boldsymbol{a}_2\boldsymbol{q}} - e^{-i\boldsymbol{a}_1\boldsymbol{q}}\right] & -3\left[e^{-i\boldsymbol{a}_2\boldsymbol{q}} + e^{-i\boldsymbol{a}_1\boldsymbol{q}}\right] & 0 & 6 \end{pmatrix}.$$

The eigenvalues of $\widehat{\mathcal{D}}$ are:

$$E_{01} = 12, \quad E_{02} = 0, \quad E_{\pm} = 6 \pm 2\sqrt{3 + 4\cos\frac{3q_x}{2}\,\cos\frac{\sqrt{3}q_y}{2} + 2\cos\sqrt{3}q_y}.$$

The expansion for small q (here $q = |\boldsymbol{q}|$) is:

$$E_- \approx \frac{3}{2}\,q^2, \quad E_+ \approx 12 - \frac{3}{2}\,q^2.$$

We find two acoustic phonons

$$\omega_{02} = 0, \quad \omega_- \approx \sqrt{\frac{3K}{8M}}\,q,$$

and two optical phonons

$$\omega_{01} \approx \sqrt{\frac{3K}{M}}, \quad \omega_+ \approx \sqrt{\frac{3K}{M}}\left(1 - \frac{q^2}{16}\right).$$

The two phonons ω_{01} and ω_{02} have no dispersion. This is an artefact of our approximation. Phonons in graphene are better described when one considers next-to-nearest neighbour couplings.