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)

A triangular lattice is a two-dimensional Bravais lattice $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2$, formed by two basis vectors $\vec{a}_1$ and $\vec{a}_2$, such that $|\vec{a}_1| = |\vec{a}_2| = a$ (a being the lattice constant). The angle between $\vec{a}_1$ and $\vec{a}_2$ is equal to $\pi/3$.

Consider a two-dimensional crystal of atoms of mass m being located in points of the Bravais lattice introduced above (one atom per unite cell). The two-dimensional displacement of an atom associated with the Bravais vector $\vec{R}_i$ is denoted by $\vec{u}_i$. The force acting on an atom associated with $\vec{R}_i$ is given by $\vec{F}_i = m\omega_0^2 \sum_j \vec{r}_{i,j}\big(\vec{r}_{i,j}\cdot(\vec{u}_j - \vec{u}_i)\big)$, where $\vec{r}_{i,j} \equiv \vec{R}_i - \vec{R}_j$ and the sum (over j) is over the nearest neighbors of $\vec{R}_i$ (there are six such neighbors).

(a) Using the Newtonian equations of motion, $m\dfrac{d^2\vec{u}_i}{dt^2} = \vec{F}_i$, determine the dispersion relation of the two acoustic phonons, i.e. the eigenfrequencies $\omega_1(\vec{k})$ and $\omega_2(\vec{k})$, where $\vec{k}$ is the wave vector.

(b) Consider the long wavelength limit, i.e., $k \to 0$, and find the velocities of the transverse and the longitudinal phonon modes.

Category B

2. Phonons in graphene (25 Points)

Consider the honeycomb lattice in graphene. Let $\mathbf{R}^{(A)}_{m,n}$ and $\mathbf{R}^{(B)}_{m,n}$ denote the positions of carbon ions in sublattices A and B, respectively, where m and n stand for the indices of a Bravais cell. The distance between neighboring ions A and B, being at equilibrium, is set to 1. We consider only nearest-neighbor couplings within the harmonic approximation for the potential. Namely, the potential energy between the 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.