

Problem Set 1

1. Monoatomic chain with longer-range interactions (2+2+2+2 points)

Consider the classical theory of lattice vibration for a monoatomic chain with periodic boundary conditions. If interactions beyond nearest-neighbors are allowed, the interaction potential is generally written as

$$V = \sum_j \sum_{l>0} \frac{1}{2} K_l (u_j - u_{j+l})^2.$$

(a) Show that the dispersion relation of the acoustic mode is given by

$$\omega_q = 2 \sqrt{\frac{1}{M} \sum_{l>0} K_l \sin^2 \frac{lqa}{2}},$$

where M is the mass of the atom and a is the lattice spacing.

(b) Show that in the long-wavelength limit the dispersion relation is given by

$$\omega_{q \rightarrow 0^+} = aq \sqrt{\frac{1}{M} \sum_{l>0} l^2 K_l},$$

provided that $\sum_{l>0} l^2 K_l$ converges.

(c) Show that if $K_l = 1/l^p$ ($1 < p < 3$), so that the sum does not converge, then in the long-wavelength limit

$$\omega_{q \rightarrow 0^+} \propto q^{(p-1)/2}.$$

Hint: For small q , the sum can be approximated by an integral, $\sum_{l=1}^{\infty} \frac{1}{l^p} \sin^2 \frac{lqa}{2} \approx (qa)^{p-1} \int_0^{\infty} dx \frac{1}{x^p} \sin^2 \frac{x}{2}$.

(d) Show that in the above long-range interacting potential with $p = 3$,

$$\omega_{q \rightarrow 0^+} \propto q \sqrt{|\ln q|}.$$

Ref: Problem 1 in Chapter 22 of Ashcroft and Mermin's book "Solid State Physics".

2. Phonons in a quantum diatomic chain (4+3+1 points)

Consider a *quantum* diatomic chain described by the Hamiltonian

$$H = \sum_{j=1}^N \sum_{\nu=1}^2 \frac{p_{j,\nu}^2}{2M_\nu} + \frac{C}{2} \sum_{j=1}^N [(u_{j,1} - u_{j,2})^2 + (u_{j,2} - u_{j+1,1})^2],$$

where M_ν are masses of the two types of atoms (labeled by $\nu = 1$ and 2) and $p_{j,\nu}$ and $u_{j,\nu}$ are momentum and displacement operators for the type- ν atom at the j -th unit cell. The distance between two neighboring atoms is $a/2$ (i.e., the same type of atoms from neighboring unit cells have distance a).

(a) Show that the Hamiltonian can be diagonalized as

$$H = \sum_q \sum_{\alpha=+,-} \hbar \omega_{q,\alpha} (b_{q,\alpha}^\dagger b_{q,\alpha} + \frac{1}{2}),$$

where the dispersion relations of the acoustic and optical phonons are given by

$$\omega_{q,\pm} = \sqrt{\frac{C}{M_1 M_2} (M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos(qa)})}.$$

Hint: Rescale and use Fourier transformation of $p_{j,\nu}$ and $u_{j,\nu}$ (periodic boundary condition assumed), diagonalize the 2×2 dynamical matrix in the Fourier space, and use the bosonic representation to diagonalize the Hamiltonian.

(b) Show that in the long-wavelength limit the dispersion relation of the acoustic phonon is given by

$$\omega_{q \rightarrow 0^+} = v_s q$$

with sound velocity

$$v_s = a \sqrt{\frac{C}{2(M_1 + M_2)}}.$$

Note that $2(M_1 + M_2)$ is the total mass of two atoms in a single unit cell.

(c) Plot the dispersion relations for $M_1 = 2M_2$ within the first Brillouin zone.

3. Volume of the first Brillouin zone (4 points)

For a three-dimensional crystal defined by the primitive vectors \vec{a}_1 , \vec{a}_2 and \vec{a}_3 , the volume of the primitive cell is given by

$$V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|.$$

Prove that the volume of the primitive cell for the reciprocal space is given by

$$\Omega \equiv |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)| = \frac{(2\pi)^3}{V}.$$

Note that Ω is also the volume of the first Brillouin zone (why?). What happens for a two-dimensional crystal?