Posted: 09.04.2019
Tutorial: 11.04.2019
Due: 25.04.2019

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

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

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

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

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

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

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

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

2. **Phonons in a quantum diatomic chain** (3+2+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 different atoms (labeled by $\nu = 1, 2$), $p_{j,\nu}$ and $u_{j,\nu}$ momentum and position (displacement) operators for the ν-th atom at the unit cell labeled by j. The distances between two neighboring atoms are $a/2$ (i.e., the ν-th 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: Use Fourier transformation of $p_{j,\nu}$ and $u_{j,\nu}$ (i.e., periodic boundary condition assumed), diagonalize the 2×2 dynamical matrix in the Fourier space, and use the bosonic realization to diagonalize the Hamiltonian.

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

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

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. **Thermal and quantum fluctuations in a harmonic oscillator** (2+2 points)

Consider a quantum harmonic oscillator described by the Hamiltonian $H = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 x^2$.

(a) Calculate $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ in the ground state $|0\rangle$, where we have defined the ground-state average of an operator A as $\langle A \rangle \equiv \langle 0|A|0\rangle$. Note that this quantity characterizes the width (i.e. quantum fluctuations) of the ground state in the real space.

(b) Calculate $\Delta x = \sqrt{\langle x^2 \rangle_T - \langle x \rangle_T^2}$ at finite temperature T, where the thermal average of an operator A is defined by $\langle A \rangle_T \equiv \frac{1}{Z}\mathrm{Tr}(Ae^{-\beta H})$ ($\beta = 1/k_B T$) with partition function $Z = \mathrm{Tr}(e^{-\beta H})$. How does Δx behave in the two different limits $k_B T \ll \hbar\omega$ and $k_B T \gg \hbar\omega$?