

Exercises for Physics 560A

Problem Set 3; Due Friday, September 23

1) Phonons in 3D

Verify that if the Fourier variables for phonons in a 3D Bravais lattice are defined by

$$Q_{\mathbf{k}\nu} = \epsilon_{\mathbf{k}\nu} \cdot N^{-1/2} \sum_{n=1}^N e^{-i\mathbf{k}\cdot\mathbf{R}_\ell} \mathbf{x}_\ell,$$
$$P_{\mathbf{k}\nu} = \epsilon_{\mathbf{k}\nu} \cdot N^{-1/2} \sum_{n=1}^N e^{i\mathbf{k}\cdot\mathbf{R}_\ell} \mathbf{p}_\ell,$$

then the displacement and momentum operators for the ℓ th atom are

$$\mathbf{x}_\ell = N^{-1/2} \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}\nu} Q_{\mathbf{k}\nu} e^{i\mathbf{k}\cdot\mathbf{R}_\ell},$$
$$\mathbf{p}_\ell = N^{-1/2} \sum_{\mathbf{k}\nu} \epsilon_{\mathbf{k}\nu} P_{\mathbf{k}\nu} e^{-i\mathbf{k}\cdot\mathbf{R}_\ell}.$$

b) The corresponding creation and annihilation operators are

$$a_{\mathbf{k}\nu} = \sqrt{\frac{m\omega_{\mathbf{k}\nu}}{2\hbar}} Q_{\mathbf{k}\nu} + \frac{iP_{-\mathbf{k}\nu}}{\sqrt{2m\hbar\omega_{\mathbf{k}\nu}}},$$
$$a_{\mathbf{k}\nu}^\dagger = \sqrt{\frac{m\omega_{\mathbf{k}\nu}}{2\hbar}} Q_{-\mathbf{k}\nu} - \frac{iP_{\mathbf{k}\nu}}{\sqrt{2m\hbar\omega_{\mathbf{k}\nu}}}.$$

Show that

$$[a_{\mathbf{k}\nu}, a_{\mathbf{k}'\nu'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\nu\nu'}.$$

2) Two-dimensional Debye model

Repeat the steps in the derivation of the Debye model for a two-dimensional crystal, assuming there are only two acoustic modes (one longitudinal and one transverse in-plane) with frequencies

$$\omega_s(\mathbf{k}) = v|\mathbf{k}|, \quad s = 1, 2,$$

where v is the speed of sound.

a) Determine the Debye frequency and the phonon density of states.

- b) Write down a general expression for the thermal average energy of the system.
- c) Show that the specific heat obeys a T^2 law in two dimensions.

3) Thermal fluctuations of a 2D crystal

Using the formalism from problem 1, calculate the mean-square displacement of an atom in the two-dimensional crystal of problem 2. Show that $\langle \mathbf{x}_i^2 \rangle \rightarrow \infty$ for $T > 0$.