1 Acoustic Phonons

To make more concrete contact with a solid, we consider a general pairwise potential of interaction between ions:

$$V_{ion} = \sum_{i<j} V(\mathbf{R}_i - \mathbf{R}_j). \tag{1}$$

The equilibrium positions, $\mathbf{R}_i^0$,of the ions are determined by the condition that the net force on each ion vanishes:

$$\mathbf{F}_j = \sum_i \nabla V(\mathbf{R}_i^0 - \mathbf{R}_j^0) = 0. \tag{2}$$

Consequently, we represent the actual position of each ion

$$\mathbf{R}_i = \mathbf{R}_i^0 + \mathbf{Q}_i \tag{3}$$

by an expansion about the equilibrium positions. Here $\mathbf{Q}_i$ plays the role of x_i in the linear chain, as they represent the displacement of each ion from its home position. The vanishing of the forces on each ion at the home positions guarantees that the Taylor expansion for the ion potential

$$V_{ion} = \sum_{i<j} V(\mathbf{R}_i^0 - \mathbf{R}_j^0) + \frac{1}{2}\sum_{i<j}(\mathbf{Q}_i - \mathbf{Q}_j)_\mu(\mathbf{Q}_i - \mathbf{Q}_j)_\gamma F_{\mu\gamma}, \tag{4}$$

with

$$F_{\mu\gamma} = \frac{\partial^2}{\partial R_\mu \partial R_\gamma} V(\mathbf{R}_i^0 - \mathbf{R}_j^0), \tag{5}$$

is harmonic to lowest order in the fluctuation about the minimum, where repeated indices are summed over.

As in the 1d chain, we diagonalize this interaction by defining the collective coordinate

$$\mathbf{Q}_i(t) = \sum_{\mathbf{k},\lambda}\left(\frac{\hbar}{2MN\omega_{\mathbf{k}},\lambda}\right)^{1/2}(b_{\mathbf{k}},\lambda\lambda_{\mathbf{k}}e^{-i\omega_{\mathbf{k},\lambda}t} + b_{\mathbf{k},\lambda}^\dagger\lambda_{-\mathbf{k}}^* e^{i\omega_{\mathbf{k},\lambda}t})e^{i\mathbf{k}.\mathbf{R}_i^0}, \tag{6}$$

where $\lambda_{\mathbf{k}}$ is a polarization vector of unit length. For a longitudinal phonon, $\lambda_{\mathbf{k}}$ is parallel to $\mathbf{k}$, while $\lambda_{\mathbf{k}}$ is perpendicular to $\mathbf{k}$ for a transverse phonon. Because $\mathbf{Q}_i$ is Hermitian, we choose the polarization vectors to be purely real. With this definition of $\mathbf{Q}_i(t)$, we rewrite the ion-potential

$$V_{ion} = \sum_{i<j} V(\mathbf{R}_i^0 - \mathbf{R}_j^0) + \frac{M}{2} \sum_{\mathbf{k},\lambda} \omega_{\mathbf{k},\lambda}^2 \mathbf{Q}_{\mathbf{k},\lambda} \mathbf{Q}_{-\mathbf{k},\lambda} \tag{7}$$

in terms of the phonon or harmonic modes,$\mathbf{Q}_{\mathbf{k},\lambda}$. For acoustic phonons, $\mathbf{Q}_{\mathbf{k},\lambda}$ describes a distortion in which neighboring ions move in the same direction. These correspond to long-wavelength modes of the crystal. We will focus only on distortions of this sort. The conjugate momentum for a phonon mode is defined by computing $\mathbf{P}_i = M\dot{\mathbf{Q}}_i$, for example, in the site representation. $\mathbf{P}_i$ and $\mathbf{Q}_i$ obey the canonical commutation relations in Eq. (**??** (13) in Lec-01).