8.231 Physics of Solids I — Fall 2017
Recitation 3

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September 22, 2017

1 Phonon Bands: Lattice Vibration

We have been considering the electrons in the solids throughout the beginning of this course. From now on, we will digress a little bit to consider the property of nuclei.

Nuclei are much heavier compared with electrons. They form the lattice and normally just vibrate around their equilibrium positions. To capture the physics of lattice vibration, we model the lattice as a one-dimensional chain of masses connected by springs. The mass of the nucleus is m and the lattice constant is κ. The nuclei spacing at equilibrium is a. Here we assume there are L nuclei and take periodic boundary condition. The position of n-th nuclei is denoted as x_n.

The Lagrangian of this system is

$$L = K - V = \sum_{n=0}^{L-1} \left[\frac{m}{2} \dot{x}_n^2 - \frac{\kappa}{2} \left(x_{n+1} - x_n - a \right)^2 \right]. \tag{1}$$

The equations of motion of nuclus n is given by

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_n} - \frac{\partial L}{\partial x_n} = 0, \tag{2}$$

which is

$$m\ddot{x}_n + \kappa(2x_n - x_{n+1} - x_n) = 0. \tag{3}$$

As usual, we try to solve the motion by using ansatz $x_n = Ae^{-i(\omega t - kna)}$. The equation of motion becomes

$$\omega^2 = \frac{2\kappa}{m} \left[1 - \cos(ka) \right] = \frac{4\kappa}{m} \sin^2 \left(\frac{ka}{2} \right). \tag{4}$$

The dispersion relation is

$$\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin \left(\frac{ka}{2} \right) \right|, \tag{5}$$

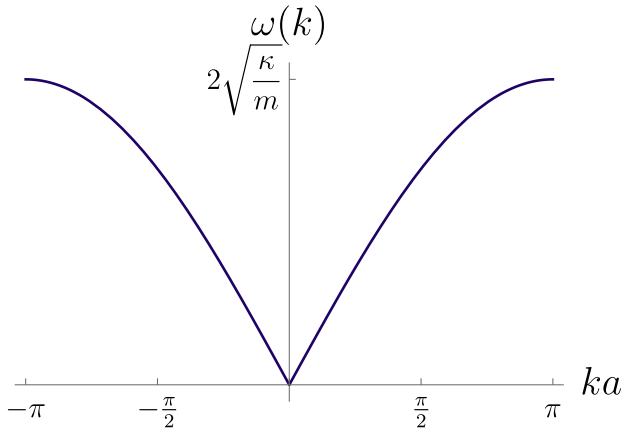

Figure 1: Dispersion of a one-dimensional harmonic chain.

It is not hard to see the possible k-mode specified by the periodic condition is the same as the one-dimensional tight-binding chain, i.e.,

$$k = \frac{2\pi m}{La}, \ m \text{ is an integer.} \tag{6}$$

Restricted to the Brillouin zone $ka \in [-\pi, \pi]$, there are exactly L different modes.

We can quantize these vibration modes. The energy eigenvalues for quantum harmonic oscillator are

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right), \ n = 0, 1, 2, \ldots. \tag{7}$$

Therefore, every given k-mode corresponds to the energy eigenstates

$$E_n(k) = \hbar\omega(k) \left(n + \frac{1}{2}\right), \ n = 0, 1, 2, \ldots. \tag{8}$$

These vibration quantum is called phonon (Greek word for "sound" or "voice"). They are responsible for properties of solids like the elasticity or sound velocity. For example, the sound velocity for long wavelength sound waves is

$$v = \left.\frac{\omega}{k}\right|_{k\to 0} = a\sqrt{\frac{\kappa}{m}}. \tag{9}$$

The reason why we consider long wavelength limit is that here unit length is a, which is the lattice spacing. This is a very small quantity (usually around a nanometer), compared with the usual sound wavelength in real life (usually several meters).

Just like electrons forming electron bands, phonons in the lattice also form bands, as shown above. Note that at band bottom, the phonon dispersion is linear while the electron dispersion is quadratic.

An important difference between phonons and electrons are that phonons are bosons. There is no Pauli exclusion principle for phonons, and each mode can be occupied by several phonons. The occupying number is determined by Bose-Einstein distribution:

$$n_{\text{B.E.}}(E) = \frac{1}{e^{E/(k_B T)} - 1}. \tag{10}$$

Also, unlike electrons, the number of phonons are not conserved. At $T = 0$, there will be no phonons—the lattice froze perfectly.