

Normal Modes of a 2D Lattice

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We now extend the method developed for a 1D lattice to two dimensions. A common system to analyze is a 2D monatomic lattice with lattice constant a in both dimensions (essentially a square Bravais lattice). For an atom of mass M at position (x_0, y_0) , a displacement in the \hat{x} direction will result in a restoring force with spring constant K_1 due to its nearest neighbors at positions $(x_0 \pm a, y_0)$ and another restoring force with spring constant K_2 due to the other two nearest neighbors at positions $(x_0, y_0 \pm a)$.

For an atom at position (na, ma) where n and m are integers, we denote its displacement from equilibrium as $u(na, ma)$. Newton's third law gives:

$$M \frac{\partial^2 u(na, ma)}{\partial t^2} = -K_1 [2u(na, ma) - u([n+1]a, ma) - u([n-1]a, ma)] \\ - K_2 [2u(na, ma) - u(na, [m+1]a) - u(na, [m-1]a)] \quad (1)$$

The Born-von Karman (periodic) boundary conditions now imply a plane wave solution:

$$u(na, ma) = Ae^{i(k_x na + k_y ma - \omega t)} \quad (2)$$

Plugging the assumed solution into the equation of motion:

$$\omega^2 = \frac{4K_1}{M} \sin^2\left(\frac{k_x a}{2}\right) + \frac{4K_2}{M} \sin^2\left(\frac{k_y a}{2}\right) \quad (3)$$

As a quick sanity check, we calculate the dispersion relation for waves propagating in the \hat{x} direction ($k_y = 0$):

$$\omega^2 = \sqrt{\frac{4K_1}{M}} \sin^2\left(\frac{k_x a}{2}\right) \quad (4)$$

which is the same result we obtained for a 1D monatomic lattice, as expected.

An interesting quantity is the velocity:

$$\mathbf{v} = \frac{\partial \omega}{\partial k_x} \hat{x} + \frac{\partial \omega}{\partial k_y} \hat{y} \quad (5)$$

$$= \frac{a}{M\omega} [K_1 \sin(k_x a) \hat{x} + K_2 \sin(k_y a) \hat{y}] \quad (6)$$

with magnitude:

$$v = \frac{a}{M\omega} \sqrt{K_1^2 \sin^2(k_x a) + K_2^2 \sin^2(k_y a)} \quad (7)$$