Dispersion relation of a one-dimensional monoatomic chain.

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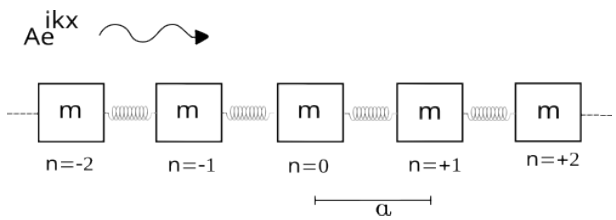
We will consider a one-dimensional crystal lattice with all atoms being equal, each with mass m, equally spaced with an atomic distance of a, and with the same elastic coupling constant α equal to 1. We can visualize this system classically as a harmonic chain of coupled masses and springs, as illustrated in Figure 1.

Figure 1: Illustration of a one-dimensional monoatomic chain with equally spaced atoms and the same elastic coupling constant.



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We define the vibrational mode as a plane wave propagating in the chain from left to right, in the form:

$$x_n = Ae^{i(kna-\omega t)}, \tag{1}$$

where A is the amplitude of the plane wave, k is the wave vector, n is the site where the atom is located, a is the atomic distance (which we will assume to be equal to 1 from now on), ω is the angular frequency, and t is the time. Taking the site $n = 0$ as the reference point, we can write the equation of motion for the mass m at the site $n = 0$ based on Newton's laws,

$$m\frac{d^2x_0}{dt^2} = \alpha(x_{-1} + x_{+1} - 2x_0). \tag{2}$$

Using the normal mode equation of the incident wave (1) in the equation of motion (2), we can arrive at the dispersion relation for the wave propagating in a one-dimensional monoatomic chain. The dispersion relation connects the frequency with the wave vector. Since the chain is one-dimensional and the wave vector dictates the direction of wave propagation, we can refer to it as the wave number.

$$m\omega^2 = 2\alpha(1 - cos(ka)). \tag{3}$$

Due to the periodicity of equation (3), since the relationship remains the same with $k \to k + 2\pi$, we can plot the dispersion relation from $-\pi$ to π.