Chapter #4:
Vibrations in a Crystal

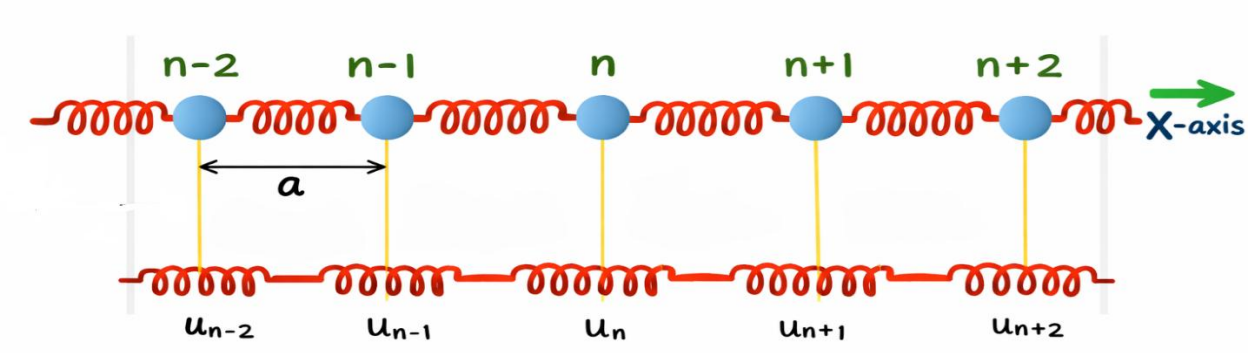
Lecture 3: Dispersion relation

In this topic, we will study the nature of vibrations inside a crystal when the wavelength of the propagating wave is comparable to the lattice constants.

(It is worth noting that if the wavelength of the propagating wave is large, then from the wave's point of view, it cannot resolve the details of the crystal structure.)

4-3 Model: 1D Monoatomic Chain

The first case we will consider is a lattice with a basis containing only one atom.



Consider a 1D chain:

The position of atoms at T = 0 K (at equilibrium) is given by: $\vec{R} = na\ \hat{x}$

Where: **n** is an integer and corresponds to a specific atom located at position R_n=na, and **a** is the lattice constant

Assume nearest-neighbor interaction:

$$\phi''_{xx}(\vec{R}-\vec{R}') = K \qquad \text{If} \quad \vec{R}-\vec{R}' = \pm a\ \hat{x}$$

$$\phi''_{xx}(\vec{R}-\vec{R}') = 0 \qquad \text{otherwise}$$

K is the effective nearest-neighbor force constant, with units of N m^{-1}. It characterizes the curvature of the interatomic potential near equilibrium.

And displacement around the equilibrium position: $\vec{u}(\vec{R}) = u(na)\,\hat{x}$

❖ Harmonic Energy of the Chain

Recall from last lecture:

$$U_{harmonic} = \frac{1}{4}\sum_R \sum_{R'} \sum_\mu \sum_\nu \frac{\partial^2 \varphi(\vec{r})}{\partial\mu\,\partial\nu}\,(u_\mu(\vec{R}) - u_\mu(\vec{R}'))\;\;(u_\nu(\vec{R}) - u_\nu(\vec{R}')) \qquad (8)$$

Then, we can rearrange this equation according to our studied case as follows:

$$U_{harmonic} = \frac{1}{4}\sum_n \sum_{n\backslash} \left[u(na) - u\,(n\backslash a)\right]^2 \varphi''_{xx}(\vec{R} - \vec{R}') \neq 0 \qquad (9)$$

If n\=n-1 and n\=n+1 for the 1st neighbors, then we will get:

$$U_{harmonic} = \frac{1}{4}\sum_n [u(na) - u((n+1)a)]^2\,K + \frac{1}{4}\sum_n [u(na) - u\,((n-1)a)]^2\,K \qquad (10)$$

If we analyze this equation, we can see that:

- Taking the 2nd term $\frac{1}{4}\sum_n [u(na) - u((n-1)a)]^2\,K$
- Choosing n\=n-1 leads to the same atom n\+1=n.
- Leading to: $\frac{1}{4}\sum_{n\backslash}\left[u(n\backslash+1)a - u(n\backslash a)\right]^2 K$
- Choosing n\=n gives us: $\frac{1}{4}\sum_n [u(n+1)a - u\,(na)]^2\,K$
- Using: $(a-b)^2 = (b-a)^2$;

$$\frac{1}{4}\sum_n [u(n+1)a - u\,(na)]^2\,K = \frac{1}{4}\sum_n [u(na) - u(n+1)a)]^2\,K$$

This is exactly identical to the first term in equation (10); therefore, we can write this equation in the following form:

$$\boxed{U_{harmonic} = \frac{1}{2}\sum_n [u(na) - u\,((n+1)a)]^2 K} \qquad (11)$$

❖ Equation of motion

Now, we will derive the equation of motion for the ion located at site n.

From Newton's law: $\vec{F} = m\vec{a} = m\frac{\partial^2 x}{\partial t^2}$

And we know that: $\vec{F} = -\vec{\nabla}U = -\frac{\partial(U_{equilibrium}+U_{harmonic})}{\partial u(na)}$

As we assumed earlier, by considering only the ***nearest neighboring atoms***, we find that:

$$U_{harmonic} = \frac{1}{2}[u((n-1)a) - u(na)]^2K + \frac{1}{2}[u(na) - u((n+1)a)]^2K + \frac{1}{2}[u((n+1)a) - u((n+2)a)]^2K$$

$$\frac{\partial U_{harmonic}}{\partial u(na)} = [u((n-1)a) - u(na)]K(-1) + [u(na) - u((n+1)a)]K(+1) + [u((n+1)a) - u((n+2)a)]K(0)$$

Accordingly, we obtain:

$$m\frac{\partial^2 u(na)}{\partial^2 t} = -\frac{\partial U_{harmonic}}{\partial u(na)} = -K[2u(na) - u((n-1)a) - u((n+1)a)] \quad (12)$$

❖ Wave Solution of the Equation of Motion

We will figure out a solution to this equation in the form of a traveling wave, where all atoms vibrate with the same frequency ω and the same amplitude A, as follows:

$$u_q(na) = Ae^{i(qna-\omega t)} \quad (13)$$

- A: displacement amplitude.
- q: wavevector in the one-dimensional chain, with units of m^{-1}.
- ω: angular frequency, with units of rad s^{-1}.
- t: time.

By substituting this solution into equation (12), we find that:

$$m\omega^2 = K[2 - e^{iqa} - e^{-iqa}] = K[2 - 2\,cos_{(qa)}]\,\omega^2 = \frac{2K}{m}[1 - cos_{(qa)}]$$

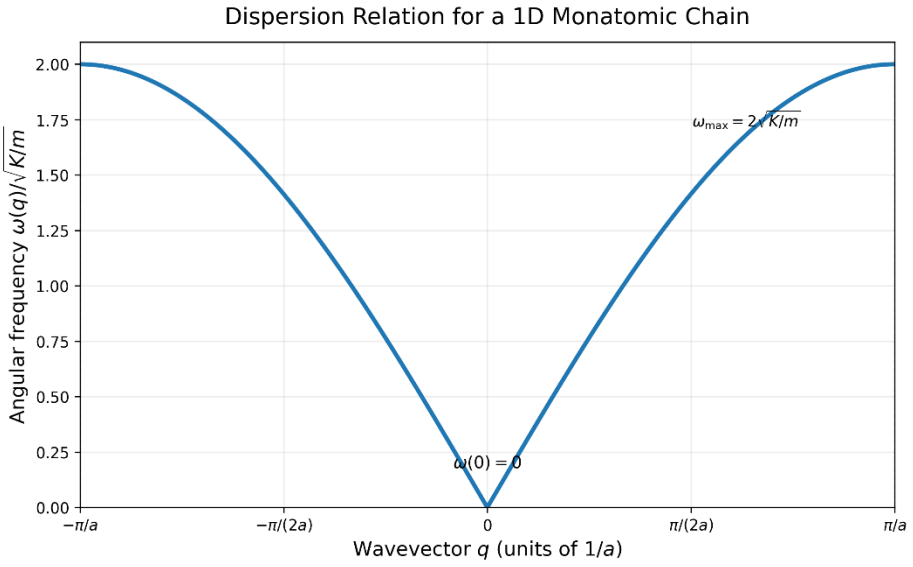
$$\because \sin^2\left(\frac{\propto}{2}\right) = \frac{1}{2}(1 - \cos \propto)$$

$$m\omega^2 = \frac{2K}{m}2\sin^2\left(\frac{\propto}{2}\right)$$

==>

$$\boxed{\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{qa}{2}\right)\right| = \omega(\vec{q})} \qquad (13)$$

This relation is called the ***dispersion relation***, as illustrated in the following figure:



- ✓ This means different wavelengths travel (q) at different speeds (ω).
- ✓ This result shows that lattice vibrations are not simple harmonic motion of individual atoms, but collective wave-like excitations.
- ✓ It defines the relationship between ω and the wave vector q.
- ✓ We can also conclude that ω depends on K, m, and q.

👉 Understanding ω(q) is essential for predicting **material behavior.**

Due to the periodicity of the crystal, we find that:

$$u_{\vec{q}}(Na) = u_{\vec{q}}(0) \qquad (14)$$

From this condition, we find that:

$$Ae^{i(qNa-\omega t)} = Ae^{-i\omega t}$$

$$e^{iqNa} = 1$$

$$qNa = 2\pi p$$

$$q = \frac{2\pi p}{Na} \qquad \text{where p is an integer.}$$

Now we will see what happens when we add $\frac{2\pi}{a}$ to q.

$$u(q + (\frac{2\pi}{a})) = Ae^{i((q+\frac{2\pi}{a})Na-\omega t)}$$

Since: $e^{i\frac{2\pi}{a}Na} = 1$

Then, $Ae^{i((q+\frac{2\pi}{a})Na-\omega t)} = u(q)$

- ✓ Thus, **q** is periodic when we add $\frac{2\pi}{a}$. Therefore, the motion of atoms with wave vector q is identical to that of atoms with wave vector $q + (\frac{2\pi p}{a})$.

Hence, the values of **q** that give independent solutions belong to the first Brillouin zone, i.e.:

$$-\pi \leq qa \leq \pi$$
$$-\frac{\pi}{a} \leq q \leq \frac{\pi}{a}$$

- ✓ Wavevectors that differ by a reciprocal-lattice vector produce the same phase pattern at the lattice sites. Therefore, it is sufficient to consider wavevectors within one first Brillouin zone.

❖ **Phase velocity:**

$$v_p = \frac{\omega}{q}$$

Since: $\omega = 2\sqrt{\frac{K}{m}}\left|\sin\ (\frac{qa}{2})\right|$

And when $qa << 1$

q

Then, $\omega = 2\sqrt{\frac{K}{m}}\frac{qa}{2}$ and $v_p = \frac{\sqrt{\frac{K}{m}}qa}{q} = \sqrt{\frac{K}{m}}a$

❖ **Group velocity:**

$$v_g = \frac{\partial \omega}{\partial q} = 2\sqrt{\frac{K}{m}}\left|cos_{(\frac{qa}{2})}\right| . \frac{a}{2}$$

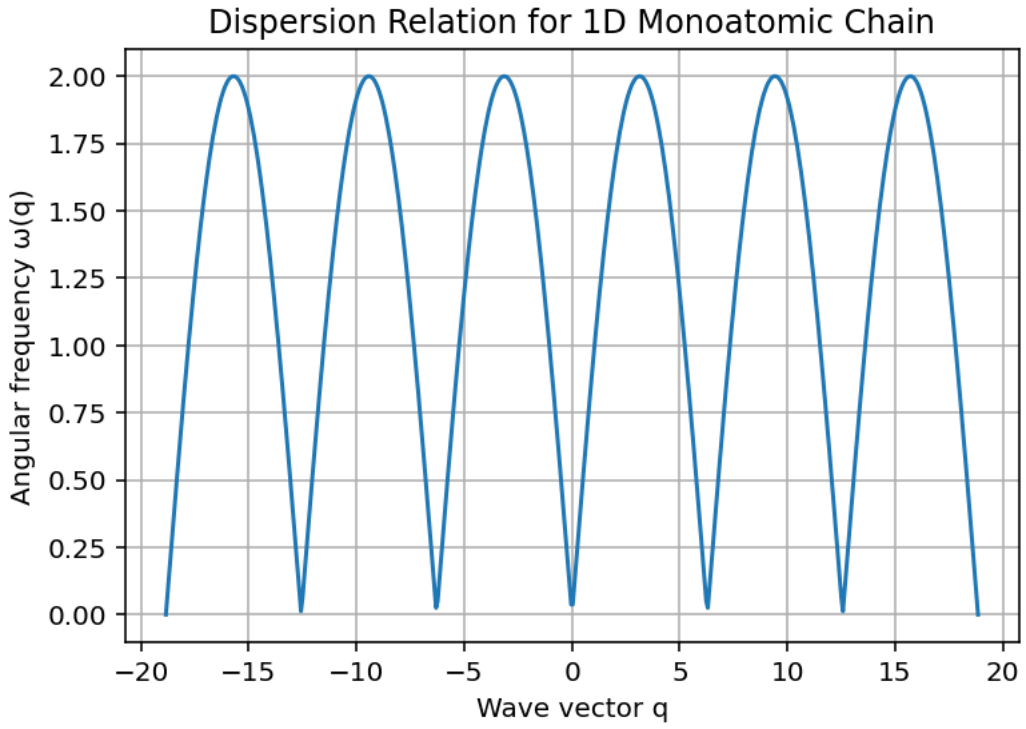
When $q = 0$, $$v_g = \frac{\partial \omega}{\partial q} = \sqrt{\frac{K}{m}}a$$

The physical difference between these two quantities is that the phase velocity (v_p) describes a pure wave with a well-defined frequency (ω) and wave vector (q), whereas the group velocity (v_g) describes the propagation of a wave packet (pulse), which has an average frequency (ω) and wave vector (q).

Since energy and momentum are, in practice, transported by wave packets rather than pure waves, the group velocity (v_g) is physically more important.

Exercise-1: Try to find (v_p) and (v_g) when ($q = \frac{\pi}{2}$) ?

Exercise 2: Try to plot the dispersion relation using Python code.




```
import numpy as np

import matplotlib.pyplot as plt
```

```
K = 1.0

m = 1.0

a = 1.0


# First Brillouin zone

q = np.linspace(-np.pi/a, np.pi/a, 10001)


omega = 2 * np.sqrt(K/m) * np.abs(np.sin(q * a / 2))


plt.figure()

plt.plot(q, omega)


# Mark Brillouin zone boundaries

plt.axvline(-np.pi/a, linestyle='--')

plt.axvline(np.pi/a, linestyle='--')

plt.axvline(0)


plt.xlabel("q")

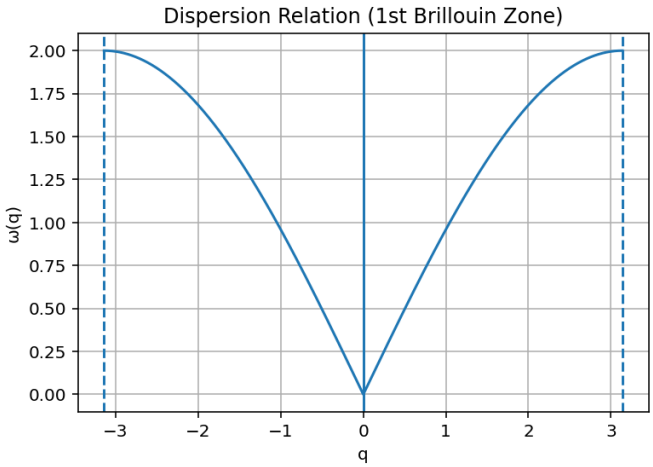
plt.ylabel("ω(q)")

plt.title("Dispersion Relation (1st Brillouin Zone)")


plt.grid()

plt.show()
```

Here, you can modify the code to cover only the 1st Brillouin zone.




```
# -*- coding: utf-8 -*-
"""
Created on Tue Apr 14 11:03:50 2026

@author: somran
"""

import numpy as np
import matplotlib.pyplot as plt

K = 1.0
m = 1.0
a = 1.0

# First Brillouin zone
```

```
q = np.linspace(-np.pi/a, np.pi/a, 10001)

omega = 2 * np.sqrt(K/m) * np.abs(np.sin(q * a / 2))

plt.figure()
plt.plot(q, omega)

# Mark Brillouin zone boundaries
plt.axvline(-np.pi/a, linestyle='--')
plt.axvline(np.pi/a, linestyle='--')
plt.axvline(0)

plt.xlabel("q")
plt.ylabel("ω(q)")
plt.title("Dispersion Relation (1st Brillouin Zone)")

plt.grid()
plt.show()
```

Student presentation:

How can we link the phase velocity and group velocity derived from vibrations with those that can be calculated using elastic constants?