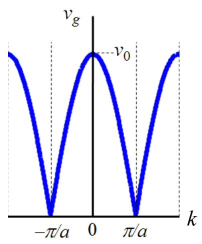
LATTICE VIBRATION

Overview: Lecture 3

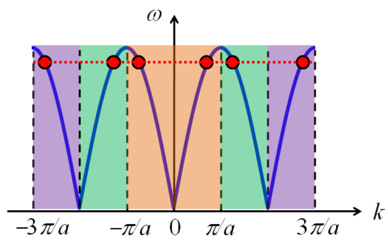
- Velocity of propagation.

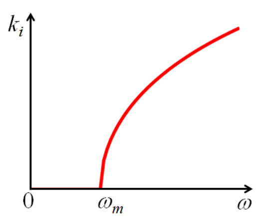
$$v_g = \frac{d\omega}{dk} = v_0 \left|\cos\frac{1}{2}ka\right|$$



- If $\omega > \omega_m$ $\rightarrow$ $k = k_r + ik_i$

- Brillouin zones $\rightarrow$ many solutions.





Overview: This Lecture

- Boundary conditions → allowed states, quantization
- Density of states
- Transverse vibration

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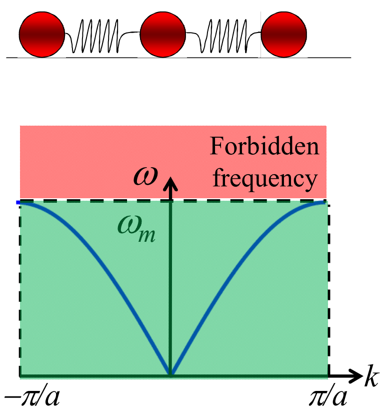
Boundary Conditions

- So far, we have an infinite possible solutions.
- Boundary conditions limit the possible frequencies or wavelengths.
- What is the number of atoms in the lattice?
  - → Very large but finite.



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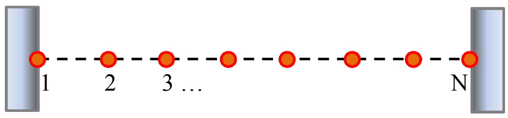
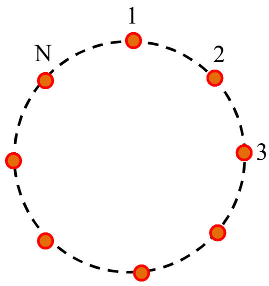
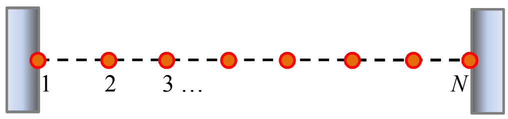
Finite Lattice Atoms

- N atoms → usually very large.
- Two commonly used boundary conditions:
  - **Fixed end:** The end atoms are clamped rigidly in place.
  - **Periodic:** The displacement of the first and last atom in the chain is assumed to be same.





Fixed End



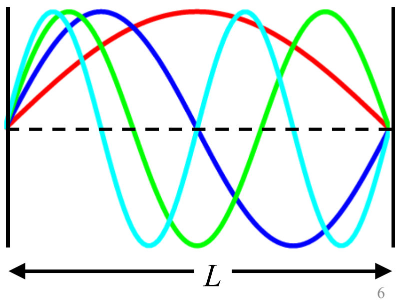
$u_1 = 0$ $\qquad$ $u_N = 0$

- Standing wave solutions:

$$u(x,t) = Ae^{ikx}e^{-i\omega t} + Ae^{-ikx}e^{-i\omega t} = (2A\cos kx)e^{-i\omega t}$$

- Not all values of k!
  - Discrete solutions.
  - $\lambda \neq 2a$.

$$\lambda = 2L, \frac{2L}{2}, \frac{2L}{3}, \cdots$$



Allowed Modes

- $\lambda = 2L, \dfrac{2L}{2}, \dfrac{2L}{3}, \cdots$
- $k = k_n = \dfrac{\pi}{L}, \dfrac{2\pi}{L}, \dfrac{3\pi}{L}, \cdots$
- $\omega_n = \omega_m \sin \dfrac{\pi}{2(N-1)}, \omega_m \sin \dfrac{2\pi}{2(N-1)}, \omega_m \sin \dfrac{3\pi}{2(N-1)}, \cdots$
- Allowed k values are equally spaced but ω values are not.

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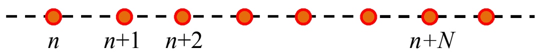
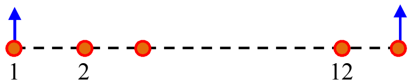
Periodic



$$u_n = u_{n+N}$$

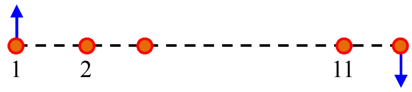
- Allows traveling waves to propagate.

- **Even number of atoms**



- $\lambda = 2a$ can be excited.

- **Odd number of atoms**



- $\lambda = 2a$ cannot be excited.

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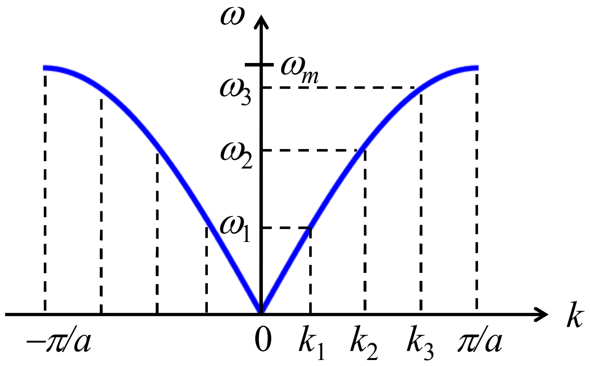
Allowed States

- Very few atoms



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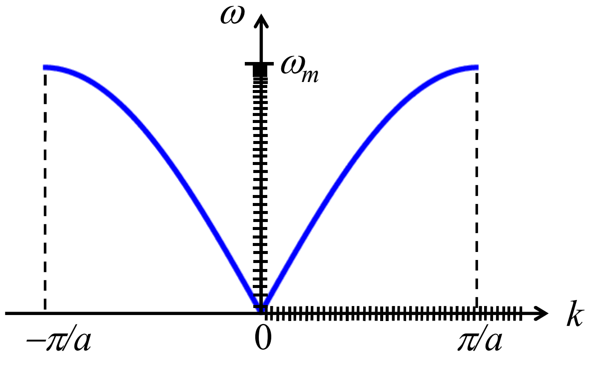
Allowed States

- Many atoms



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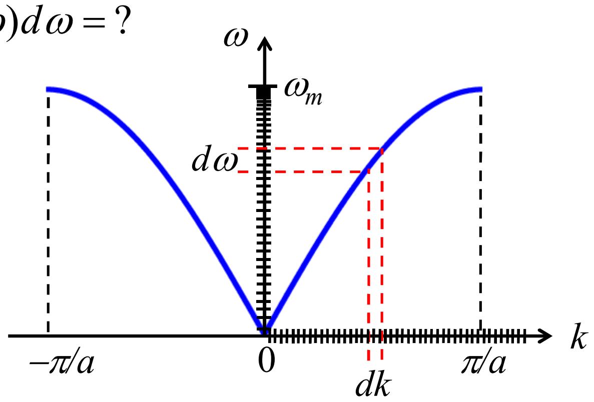
Density of States

$$g(k)dk = ?$$

$$g(\omega)d\omega = ?$$



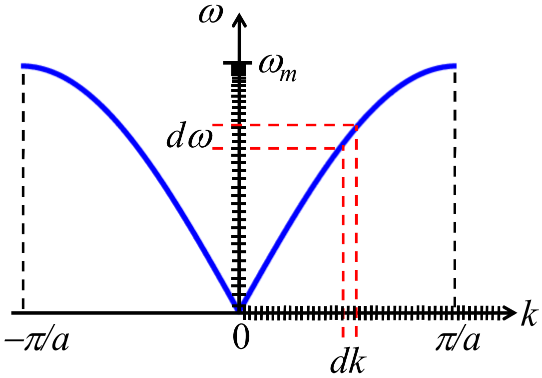
Density of States

- Since k values are equally spaced,

$$g(k)dk = \frac{N}{2\pi / a} dk = \frac{Na}{2\pi} dk$$

$$g(\omega)d\omega = g(k)dk$$

$$= \frac{Na}{2\pi} \frac{dk}{d\omega} d\omega$$



Density of States

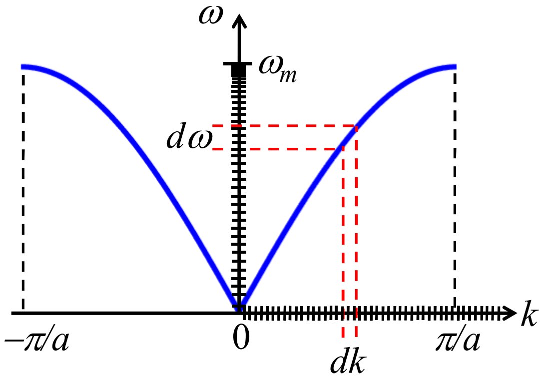
$$\omega = \omega_m \sin\frac{ka}{2} \Rightarrow \frac{d\omega}{dk} = \omega_m \frac{a}{2}\cos\frac{ka}{2}$$

$$\frac{dk}{d\omega} = \frac{2}{\omega_m a}\frac{1}{\cos(ka/2)}$$

$$g(\omega)d\omega = \frac{N}{\pi}\frac{d\omega}{\omega_m \cos(ka/2)}$$

- For small frequencies,

$$g(\omega)d\omega = \frac{N}{\pi}\frac{d\omega}{\omega_m}$$



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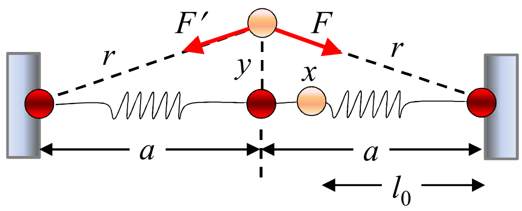
Transverse Waves

- Transverse waves are polarized.
- The velocity may differ from that of longitudinal waves.
- The force constants for longitudinal and transverse motions are different.



$$F_l = m\ddot{x} = -C_l x$$

$$F_t = m\ddot{y} = 2F\sin\theta = -C_t y$$

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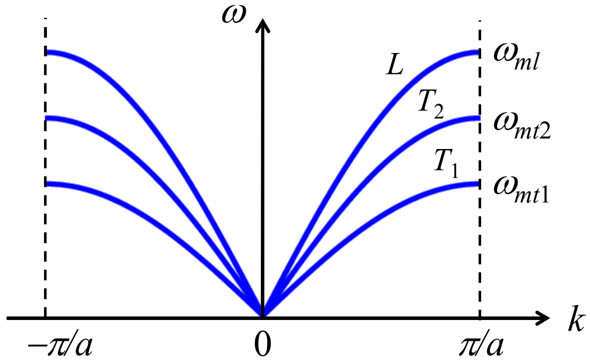
Transverse Waves

- Two mutually perpendicular transverse polarization directions.
- Two transverse modes may have different dispersion relations.



- **Dispersions:** $\omega_l = \sqrt{\frac{4C_l}{m}}\left|\sin\frac{ka}{2}\right|, \quad \omega_t = \sqrt{\frac{4C_t}{m}}\left|\sin\frac{ka}{2}\right|$

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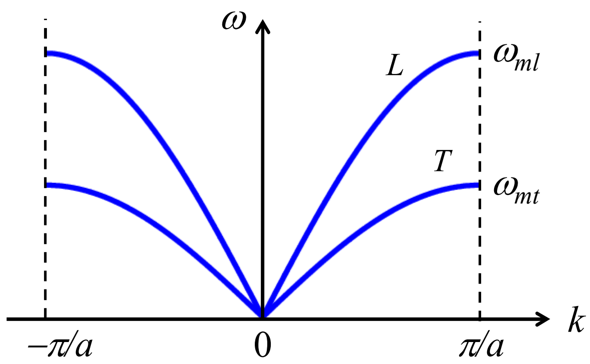
Transverse Waves

- For symmetric crystals, the transverse polarization directions and dispersion relations of two transverse modes are identical.



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