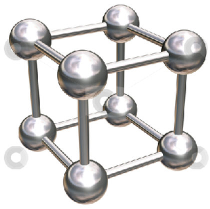
LATTICE VIBRATION

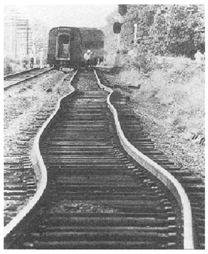
First Assignment - Reminder

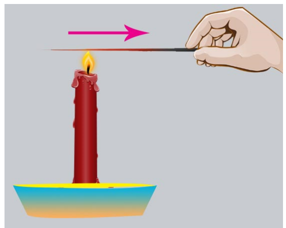
- Email to anis@eee.buet.ac.bd with
  - **Subject:** EEE 461
  - **Body:** "Your Name, Student Number" <email address>
- It will help me to keep you posted on the course updates.

Crystal Dynamics

- Elementary physics → atoms are rigidly located.
- Can we explain specific heat, thermal expansion and thermal conductivity?





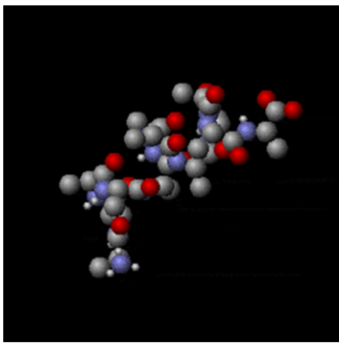


3

Harmonic Motion

- Atoms vibrate even at absolute zero around equilibrium
  → zero point motion, zero point energy.
- The amplitude of the motion increases as the atoms gain more thermal energy at higher temperatures.

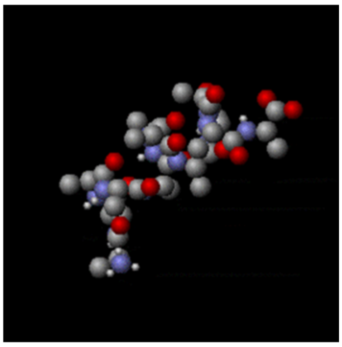
- We need a refined model.
  - Atoms are allowed to vibrate around their equilibrium positions.



4

Refined Model

- The refined model leads to
  - the conditions for wave propagation in a periodic lattice,
  - the energy content,
  - the specific heat of lattice waves,
  - the particle aspects of vibrations
  - the coupling between phonons and propagating EM waves.



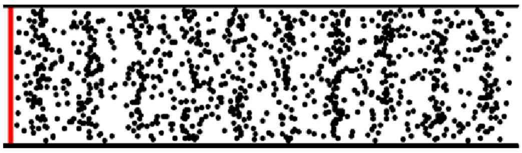
- Also introduces
  - forbidden and permitted frequency ranges, and
  - electronic spectra of solids.

5

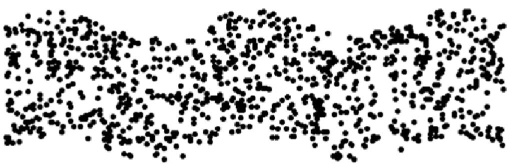
Propagating Waves

- Two basic types of wave motion: **Longitudinal** and **Transverse**.
- Often we are interested in the propagation of sound waves through crystals.

Longitudinal Waves



Transverse Waves



6

Interatomic Bonding

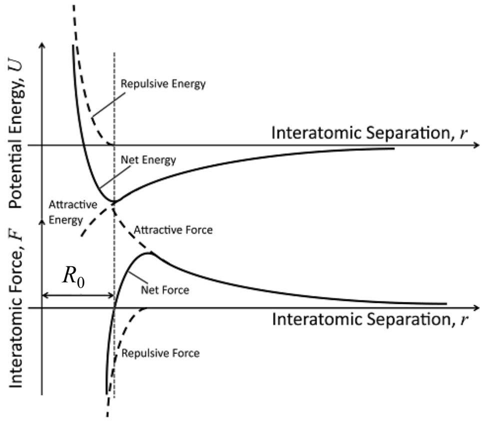
- Balance between electrostatic attractive and repulsive forces.

- **Potential energy:**

$$U = -\frac{A}{r^n} + \frac{B}{r^m}$$

- **Force:**

$$F = -\frac{dU(r)}{dr} = -\frac{nA}{r^{n+1}} + \frac{mB}{r^{m+1}}$$



- **Equilibrium:**

$$F = 0, \quad R_0 = \left(\frac{mB}{nA}\right)^{1/(m-n)}, \quad U(R_0) = -\frac{A}{R_0^n}\left(1 - \frac{n}{m}\right)$$

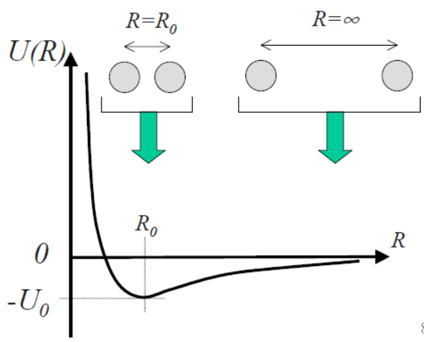
7

Vibration: Mathematical Model

- Consider 1-D system of two neighboring atoms, one at the origin ($R = 0$) and the other at a distance $R \rightarrow$ vibrating around R_0.

- $$U(R) = U(R_0) + \left(\frac{dU}{dR}\right)_{R_0}(R - R_0) + \frac{1}{2}\left(\frac{d^2U}{dR^2}\right)_{R_0}(R - R_0)^2 + \frac{1}{6}\left(\frac{d^3U}{dR^3}\right)_{R_0}(R - R_0)^3 + \cdots$$

- $$\left(\frac{dU}{dR}\right)_{R_0} = 0$$



8

Vibration: Mathematical Model

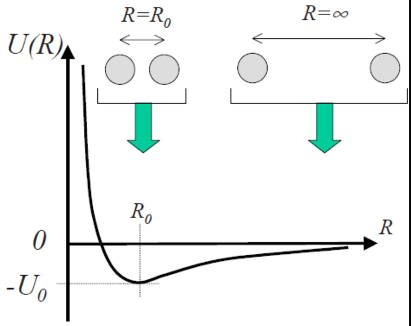
- Let $U_0 = -U(R_0)$ and $R - R_0 = x$

$$U(R) + U_0 = \frac{1}{2}C_1 x^2 + C_2 x^3 + \cdots$$

- where

$$\underbrace{C_1 = \left(\frac{d^2U}{dR^2}\right)_{R_0}, \quad C_2 = \frac{1}{6}\left(\frac{d^3U}{dR^3}\right)_{R_0}}$$

Constants, depend on the nature of the crystal formation



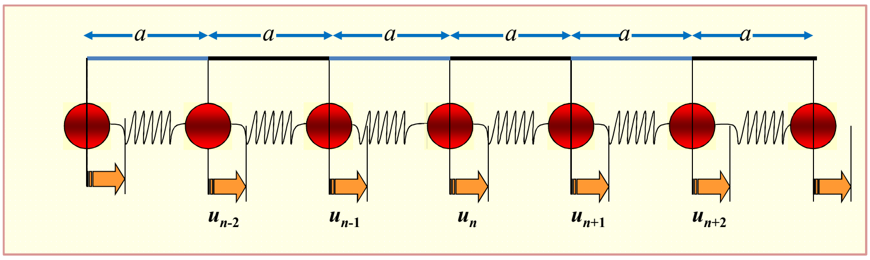
Force:

$$F = -\frac{d}{dx}\left(\frac{1}{2}C_1 x^2\right) = -C_1 x$$

9

1-D Monatomic Lattice

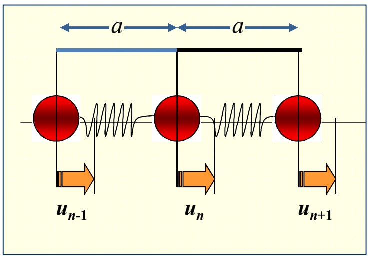
- The simplest crystal.
- Identical masses with a spacing of a.
- Atoms move only in a direction parallel to the chain.
- Consider only nearest neighbors interact (short-range forces).



10

1-D Monatomic Lattice

- Consider only nearest neighbor interactions.



The force on the *n*-th atom:

- By the $(n-1)$-th atom:

$$F_{n,n-1} = -C\left(u_n - u_{n-1}\right)$$

- By the $(n+1)$-th atom,

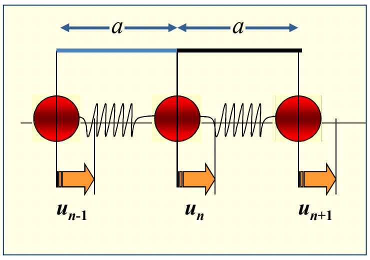
$$F_{n,n+1} = -C\left(u_n - u_{n+1}\right)$$

- C: Spring constant → Characteristic of the spring.

11

1-D Monatomic Lattice

- Consider only nearest neighbor interactions.



The resultant force on the *n*-th atom:

$$F_n = F_{n,n-1} + F_{n,n+1}$$
$$= C\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

- Using Newton's mass action law:

$$F_n = m\frac{d^2u_n}{dt^2} = C\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

- We obtain a large number of coupled differential equations.

12

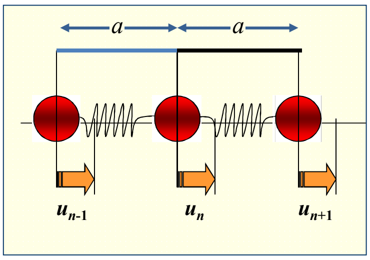
Displacement Solutions

- Traveling wave solutions:

$$u_n = Ae^{i(kx_n - \omega t)} = Ae^{i(kna - \omega t)}$$

$$u_{n+1} = Ae^{i[k(n+1)a - \omega t]} = e^{ika} u_n$$

$$u_{n-1} = Ae^{i[k(n-1)a - \omega t]} = e^{-ika} u_n$$



- After substitution in the equation of force

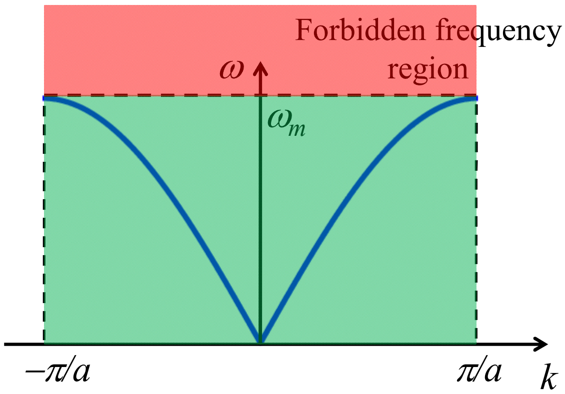
$$F_n = m\frac{d^2 u_n}{dt^2} = C\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

$$\omega^2 = \frac{C}{m}\left(2 - e^{ika} - e^{-ika}\right) = \frac{2C}{m}\left(1 - \cos ka\right) = \frac{4C}{m}\sin^2\frac{ka}{2}$$

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{ka}{2}\right| = \omega_m\left|\sin\frac{ka}{2}\right|$$

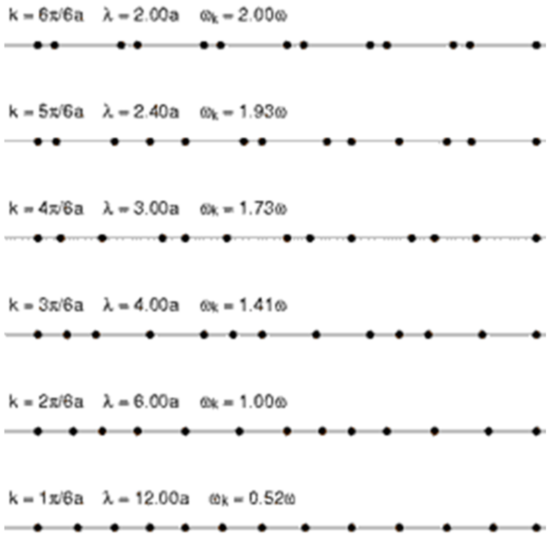
Dispersion

$$\omega = \omega_m\left|\sin\frac{ka}{2}\right|$$



- The system is dispersive.
- There is an upper limit of $\omega_m \rightarrow$ low-pass filter.
- Transverse waves behave similar.

ω vs. k


k = 6π/6a λ = 2.00a ωk = 2.00ω
k = 5π/6a λ = 2.40a ωk = 1.93ω
k = 4π/6a λ = 3.00a ωk = 1.73ω
k = 3π/6a λ = 4.00a ωk = 1.41ω
k = 2π/6a λ = 6.00a ωk = 1.00ω
k = 1π/6a λ = 12.00a ωk = 0.52ω

15