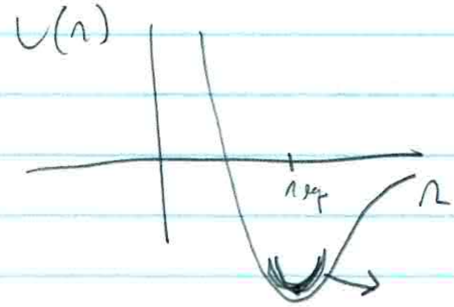
Lecture #11: Classical description of lattice vibrations

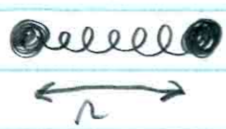


Close to $r = r_{eq}$, we can always expand $U(r) \approx U(r_{eq}) + \frac{1}{2}\left.\frac{d^2U}{dr^2}\right|_{r=r_{eq}} (r - r_{eq})^2$

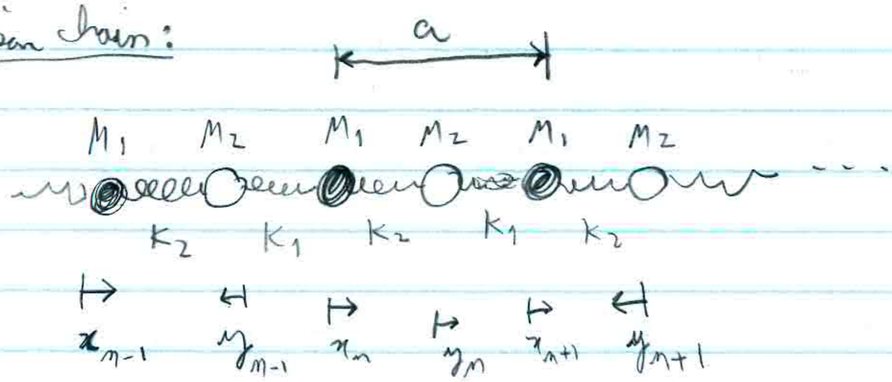
$+ \mathcal{O}(r - r_{eq})^3$

$$\Rightarrow U(r) \approx U(r_{eq}) + \frac{1}{2} K r^2$$

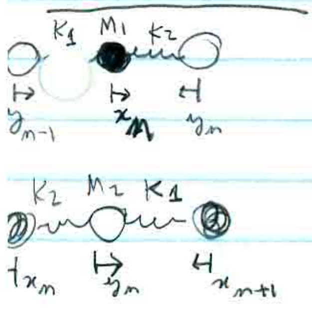
"Hooke's law".



Linear chain:



Newton's law:



$$\begin{cases} M_1 \ddot{x}_n = K_2 (y_n - x_n) + K_1 (y_{n-1} - x_n) \\ M_2 \ddot{y}_n = K_1 (x_{n+1} - y_n) + K_2 (x_n - y_n) \end{cases}$$

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Guess a solution of the form:

$$\begin{cases} x_n(t) = x_0 e^{i(kan - \omega t)} \\ y_n(t) = y_0 e^{i(kan - \omega t)} \end{cases}$$

Plug into the EOMs:

$$\begin{cases} -M_1 \omega^2 x_0 = K_2 (y_0 - x_0) + K_1 \left(y_0 e^{-ika} - x_0 \right) \\ -M_2 \omega^2 y_0 = K_1 (x_0 e^{ika} - y_0) + K_2 (x_0 - y_0) \end{cases}$$

$$\Rightarrow \begin{pmatrix} -\frac{(K_1 + K_2)}{M_1} & +\frac{K_1 e^{-ika} + K_2}{M_1} \\ \frac{K_1 e^{ika} + K_2}{M_2} & -\frac{(K_1 + K_2)}{M_2} \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = -\omega^2 \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}$$

Non zero solutions if

$$\frac{1}{M_1 M_2} \left[-(K_1 + K_2) + M_1 \omega^2 \right] \left[-(K_1 + K_2) + M_2 \omega^2 \right] - \frac{1}{M_1 M_2} \left[(K_1 e^{-ika} + K_2)(K_1 e^{ika} + K_2) \right] = 0$$

$$(K_1 + K_2)^2 + M_1 M_2 \omega^4 - (K_1 + K_2) \omega^2 (M_1 + M_2) - (K_1^2 + K_2^2) - 2 K_1 K_2 \cos(ka) = 0$$

$$\boxed{\omega^4 - \frac{(M_1 + M_2)}{M_1 M_2} (K_1 + K_2) \omega^2 + 2 \frac{K_1 K_2}{M_1 M_2} \left[1 - \cos(ka) \right] = 0}$$

$$\omega_{\pm}^2 = \frac{1}{2} \left\{ \left(\frac{M_1 + M_2}{M_1 M_2} \right) (K_1 + K_2) \pm \sqrt{ \left(\frac{M_1 + M_2}{M_1 M_2} \right)^2 (K_1 + K_2)^2 - \frac{8 K_1 K_2}{M_1 M_2} \underbrace{\left[1 - \cos(ka) \right]}_{2 \sin^2 \left(\frac{ka}{2} \right)} } \right\} //$$

two branches, ω_+ and ω_-:

$$\omega_\pm^2 = \frac{1}{2}\left(\frac{M_1+M_2}{M_1M_2}\right)(K_1+K_2)\left[1 \pm \sqrt{1 - \frac{16\,M_1M_2}{(M_1+M_2)^2}\frac{K_1K_2}{(K_1+K_2)^2}\sin^2\left(\frac{ka}{2}\right)}\right]$$

At low k: $(ka) \ll 1$:

$$\omega_\pm^2 \approx \frac{1}{2}\left(\frac{M_1+M_2}{M_1M_2}\right)(K_1+K_2)\left[1 \pm \left(1 - \frac{8\,M_1M_2}{(M_1+M_2)^2}\frac{K_1K_2}{(K_1+K_2)^2}\frac{(ka)^2}{4}\right) + \mathcal{O}(ka)^4\right]$$

$$\omega_+^2 \approx \frac{M_1+M_2}{M_1M_2}(K_1+K_2)$$

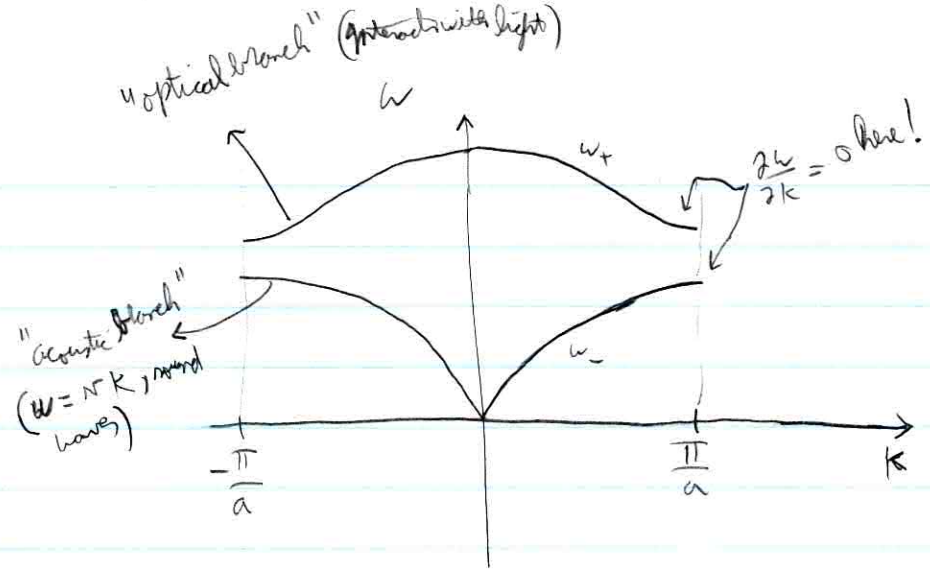
$$\omega_-^2 \approx \frac{1}{\cancel{2}}\cancel{\left(\frac{M_1+M_2}{M_1M_2}\right)}\cancel{(K_1+K_2)}\left[\frac{\cancel{8}\,\cancel{M_1M_2}}{(M_1+M_2)^2}\frac{K_1K_2}{(K_1+K_2)^2}\frac{(ka)^2}{\cancel{4}}\right] + \mathcal{O}(ka)^4$$

$$\omega_-^2 \approx \frac{K_1K_2}{(M_1+M_2)(K_1+K_2)}(ka)^2$$

$\underline{ka \ll 1:}$

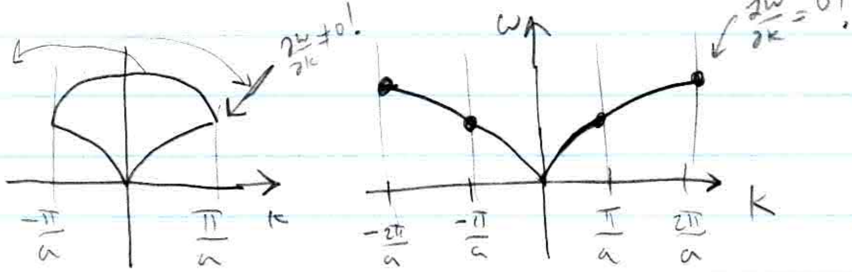
$$\Rightarrow \quad \omega_+ \approx \sqrt{\frac{\overbrace{(K_1+K_2)}^{\text{Two springs in parallel}}}{\underbrace{\left(\frac{M_1M_2}{M_1+M_2}\right)}_{\text{reduced mass!}}}}$$

$$\omega_- \approx \sqrt{\frac{\overbrace{\frac{K_1K_2}{(K_1+K_2)}}^{\text{Two springs in series}}}{(M_1+M_2)}}\,(ka)$$



Note: $\omega_\pm$ depends only on $\cos(ka)$, so k is mod $\frac{2\pi}{a}$, just like the electronic band structure!
"Reduced zone scheme".

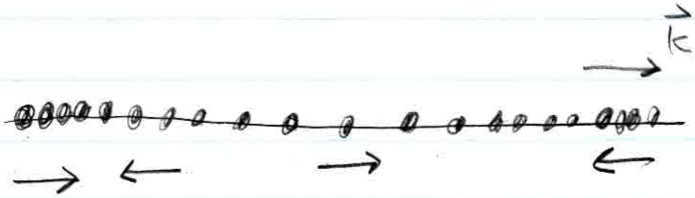
When $M_1 = M_2$ and $K_1 = K_2$:



Higher dimension ($d=3$)

Monatomic lattice:

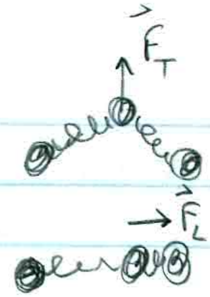
Pure transverse wave



Pure longitudinal wave

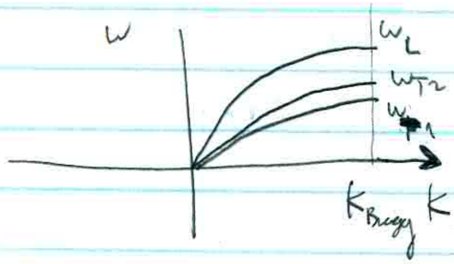
For each $\vec{k}$, there are 3 modes (because there are 3 spatial dimensions). Two are transverse and 1 is longitudinal.

Usually $\omega_L > \omega_T$ (Because it's easier to displace a spring like that



$\vec{F}_L > \vec{F}_T$)

Also, when $\vec{k} \to 0$ the atomic motions are global translations. Hence, $\vec{\omega}(\vec{k} \to 0) \to 0$.



"Acoustic modes", because $\omega = v k$

<u>Multiatomic lattice</u>: s atoms per unit cell

- Total # of degrees of freedom: $3N s$
  N ↓ # of unit cells

(N unit cells in Bravais ⇒

- N states ($\vec{k}$'s) within 1st Brillouin zone (due to periodic Bound. conds.); Hence # of branches is

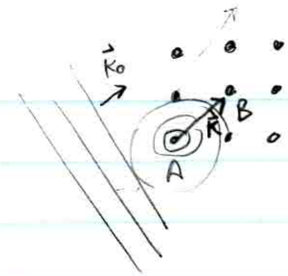
$$\frac{3Ns}{N} = 3s \;//$$

- Total # of acoustic branches $\left(\begin{smallmatrix}\omega \to 0 \\ \vec{k} \to 0\end{smallmatrix}\right)$ ⇒ 3 // (3 directions for global translations)

- Total # of optical branches $\left(\begin{smallmatrix}\omega \not\to 0 \\ \vec{k} \to 0\end{smallmatrix}\right)$ $3(s-1)$. //

<u>Neutron scattering</u> ⇓ Continue here on Friday Oct 22!

neutrons have mass but don't have charge. Hence when a beam of neutrons hits a solid it excites lattice vibrations. Inelastic neutron scattering is a great tool to map out the dispersion of lattice waves.



Neutron scatters off at A and reaches B:

$$A = e^{i\vec{k}_0\cdot\vec{R}_B} + e^{i\vec{k}\cdot\vec{R}_B}$$
$$= e^{i\vec{k}_0\cdot\vec{R}_B}\left(1 + e^{i\underbrace{\vec{s}}_{(\vec{k}-\vec{k}_0)}\cdot\vec{R}_B}\right)$$
$$A_{Total} = \sum_B \left(1 + e^{i\vec{s}\cdot\vec{R}_B}\right)$$

Like for X-ray scattering,

$$A_{sum} = \sum_l e^{i\vec{s}\cdot\vec{r}_l} e^{-i\omega t}$$

$$\vec{s} = \left(\vec{k} - \vec{k}_0\right)$$

The displacement of a given atom is given by

$$\vec{u}_l = \vec{u}_l^{(0)} e^{i\left(\vec{q}\cdot\vec{r}_l - \omega_{\vec{q}} t\right)}$$

$$A_{sum} = \sum_l e^{i\vec{s}\cdot(\vec{r}_l + \vec{u}_l)} e^{-i\omega t}$$

$$e^{i\vec{s}\cdot\vec{u}_l} \approx 1 + i\vec{s}\cdot\vec{u}_l$$

$$A_{sum} \approx \underbrace{\sum_l e^{i\vec{s}\cdot\vec{r}_l} e^{-i\omega t}}_{A_{elast},\ \text{elastic scattering}} + \underbrace{i\vec{s}\cdot\sum_l \vec{u}_l e^{i\vec{s}\cdot\vec{r}_l} e^{-i\omega t}}_{A_{inel},\ \text{inelastic scattering}}$$

$$A_{inel.} = i\vec{s}\cdot\vec{u}_l^{(0)} \sum_l e^{i\underbrace{(\vec{s}+\vec{q})}_{\text{Momentum is now } \vec{k}+\vec{q}}\cdot\vec{r}_l} e^{-i\underbrace{(\omega + \omega_{\vec{q}})}_{\text{frequency (energy) increased by } \omega_{\vec{q}}} t}$$

$\Rightarrow$ Lattice vibration got "absorbed" by neutrons.

Resonance occurs when:

$$\Longrightarrow \left(\vec{s} + \vec{q}\right) = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3 = \text{Reciprocal lattice vector}$$

If we know the reciprocal lattice vector, we can deduce $\vec{q}$

Also, $\Delta E = \hbar\omega_{\vec{q}} = \dfrac{\hbar^2 k^2}{2M_{neutron}} - \dfrac{\hbar^2 k_0^2}{2M_{neutron}}$

$\Rightarrow$ If we measure the energy gained/lost by neutron beam, we can deduce $\omega_{\vec{q}}$!