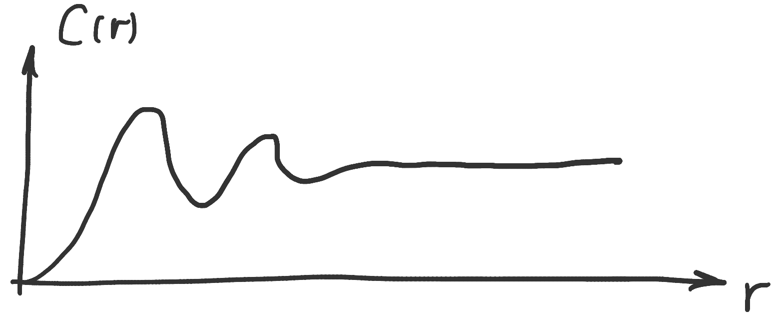
Phonons in solids I

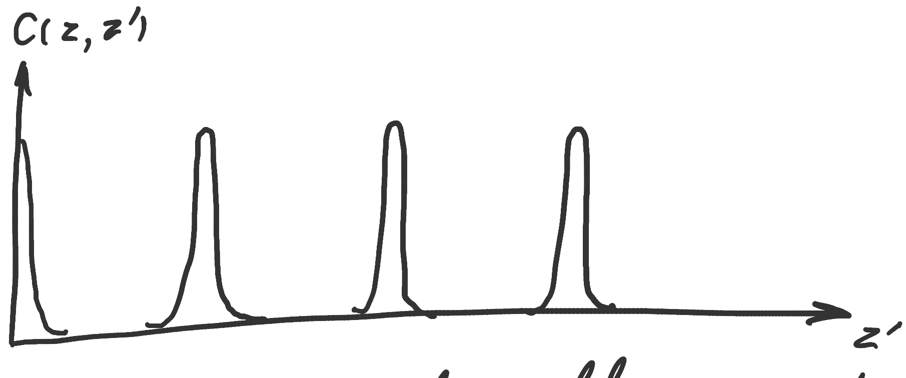
Solids - in equilibrium atoms only vibrate slightly around equilibrium positions

$$\langle n(\vec{r})\, n(\vec{r}\,')\rangle = C(\vec{r}, \vec{r}\,')$$

In liquids and gases $C(\vec{r}, \vec{r}\,') = C(\vec{r} - \vec{r}\,')$



In solid state there is long-range order



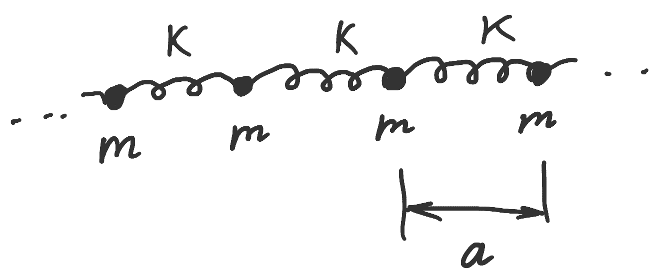
A solid in thermal equilibrium must be crystalline. Atoms tend to minimise their ... Temperature $T <$ Interaction

<u>crystalline</u>. Atoms [illegible] potential energy. Temperature T < Interaction energy.

Amorphous solids and glasses — not in equilibrium.

In addition to the positions of the atoms, there may be other degrees of freedom (spins, dipole moments)

<u>Vibrations in a 1D crystal</u>



$$H = \sum_i \left[\frac{p_i^2}{2m} + K(x_i - x_{i+1})^2 \right]$$

The Hamilton's equations:

$$\begin{cases} \dot{x}_i = \dfrac{\partial H}{\partial p_i} \\ \dot{p}_i = -\dfrac{\partial H}{\partial x_i} \end{cases}$$

$$\begin{cases} \dot{x}_i = \dfrac{p_i}{m} \\ \dot{p}_i = -K(x_i - x_{i+1}) - K(x_i - x_{i-1}) \end{cases}$$

$$m\ddot{x}_i = K(x_{i+1} + x_{i-1} - 2x_i)$$

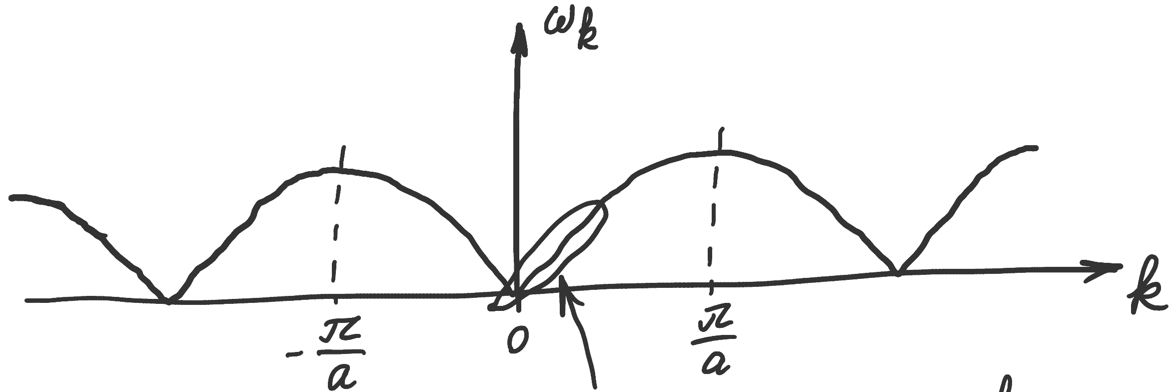
[illegible] $x = Ae^{i(kna-\omega t)}$

$$m\ddot{x}_i = K(x_{i+1} + x_{i-1} - 2x_i)$$

Look for the solution in the form $x_n = Ae^{i(kna-\omega t)}$

$$-m\omega^2 = K(e^{ika} + e^{-ika} - 2)$$

$$\omega^2 = \frac{2K}{m}(1-\cos(ka)) = \frac{4K}{m}\sin^2\frac{ka}{2}$$



At small k

$$\omega \simeq a\sqrt{\frac{K}{m}}\,k = sk$$

$$\omega \simeq a\sqrt{\frac{K}{m}}\,k$$

$s = a\sqrt{\frac{K}{m}}$ – speed of sound

Note: the wavevector is defined up to $\frac{2\pi}{a}$.

Indeed, because a wave has the form $X_k \propto e^{ikna}$, adding $\frac{2\pi}{a}$ to the wavevector k does not change anything

$$k \longleftrightarrow k + \frac{2\pi}{a}$$ – indistinguishable wavevectors

Therefore, it is enough to consider wavevectors from any interval of k of the width $\frac{2\pi}{a}$

Therefore, it is enough to consider waves $\frac{2\pi}{a}$
confined to any interval of k of the width

$\left(-\frac{\pi}{a};\ \frac{\pi}{a}\right)$ – 1-st Brillouin zone

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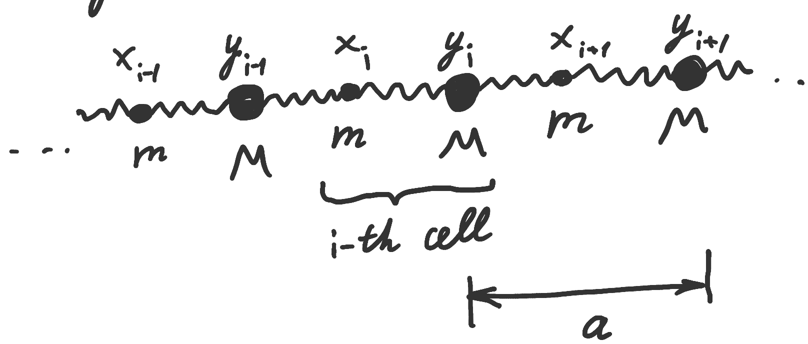
In reality there are several atoms in the elementary cell



$$\begin{cases} m\ddot{x}_i = -K(x_i - y_i) - K(x_i - y_{i-1}) \\ M\ddot{y}_i = -K(y_i - x_i) - K(y_i - x_{i+1}) \end{cases}$$

$$\begin{cases} m\ddot{x}_i = K(y_i + y_{i-1} - 2x_i) \\ M\ddot{y}_i = K(x_i + x_{i+1} - 2y_i) \end{cases}$$

Look for the solution in the form

$$x_n = x_k\, e^{i(kna - \omega t)}, \quad y_n = y_k\, e^{i[ka(n+\frac{1}{2}) - \omega t]}$$

$$\begin{cases} m\omega^2 x_k = 2K\, x_k - 2K\cos\frac{ka}{2}\cdot y_k \\ M\omega^2 y_k = 2K\, y_k - 2K\cos\frac{ka}{2}\cdot x_k \end{cases}$$

2 Equations for 2 variables x_k and y_k

... a solution

2 Equations for 2 variables x_k

$x_k = y_k = 0$ is a solution

Non-trivial solutions exist if $\det = 0$

$$\det \begin{pmatrix} 2K - m\omega^2 & -2K\cos\frac{ka}{2} \\ -2K\cos\frac{ka}{2} & 2K - M\omega^2 \end{pmatrix} = 0$$

$$Mm\,\omega^4 - 2\omega^2 K(M+m) + 4K^2 - 4K^2\cos^2\frac{ka}{2} = 0$$

Introduce the reduced mass $\mu = \dfrac{Mm}{M+m}$

$$\omega^4 - \frac{2K}{\mu}\omega^2 + \frac{4K^2}{mM}\sin^2\frac{ka}{2} = 0$$

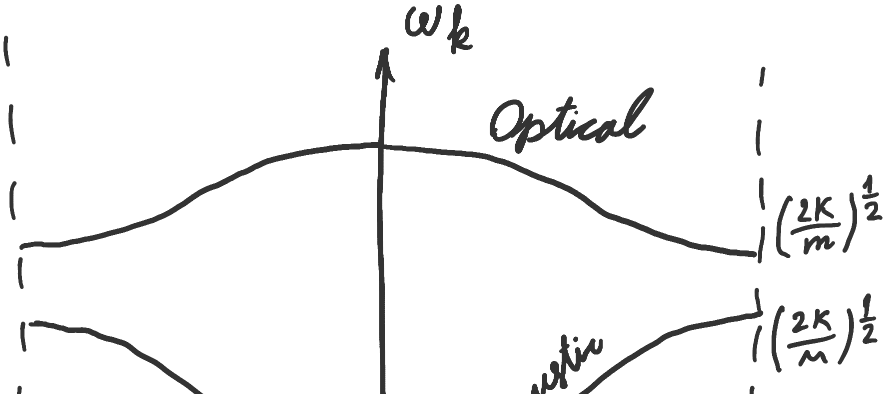
$$\omega_\pm^2(k) = \frac{K}{\mu}\left(1 \pm \sqrt{1 - \frac{4\mu^2}{mM}\sin^2\frac{ka}{2}}\right)$$

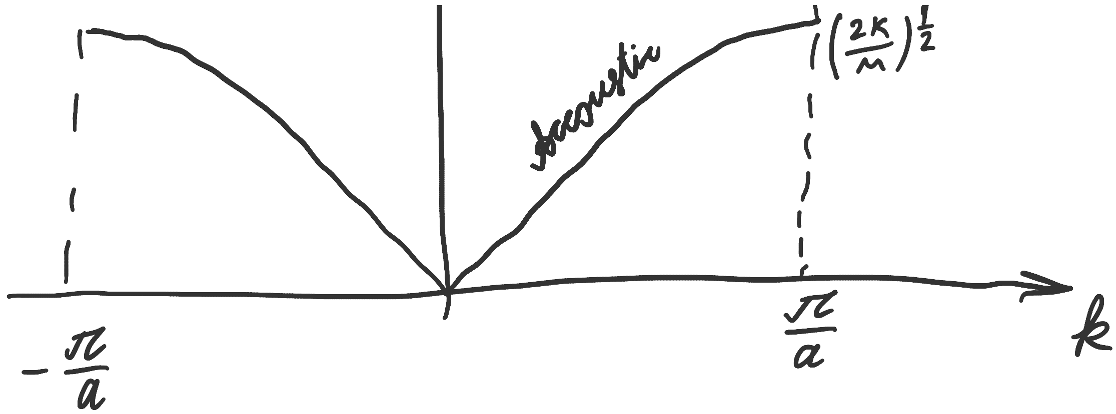
2 branches !!

In the limit $k \to 0$

$$\omega_-^2(k) = \frac{2K\mu}{mM}\left(\frac{ka}{2}\right)^2$$

$$\omega_-(k) = sk \quad \text{with} \quad s = \frac{1}{2}\left(\frac{2K}{M+m}\right)^{\frac{1}{2}}$$





Find the gap.

$$1-\frac{4\mu^2}{mM}=1-\frac{4Mm}{(M+m)^2}=\frac{(M-m)^2}{(M+m)^2}$$

The maximum of the accoustic branch:

$$\omega_-^2\left(\frac{\pi}{a}\right)=\frac{K}{\mu}\left(1-\frac{M-m}{M+m}\right)=\frac{2K}{M}$$

The minimum of the optical branch:

$$\omega_+\left(\frac{\pi}{a}\right)=\frac{K}{\mu}\left(1+\frac{M-m}{M+m}\right)=\frac{2K}{m}$$

The dispersion of the optical branch at small k:

$$\omega_+(k)\approx\sqrt{\frac{2K}{m}}\left(1+\frac{m}{2M}\cos^2\frac{ka}{2}+O\left(\frac{m^2}{M^2}\right)\right)$$

In the limit $m \ll M$ the dispersion is flat; this corresponds to the vibrations of the light atoms between the heavy ones.