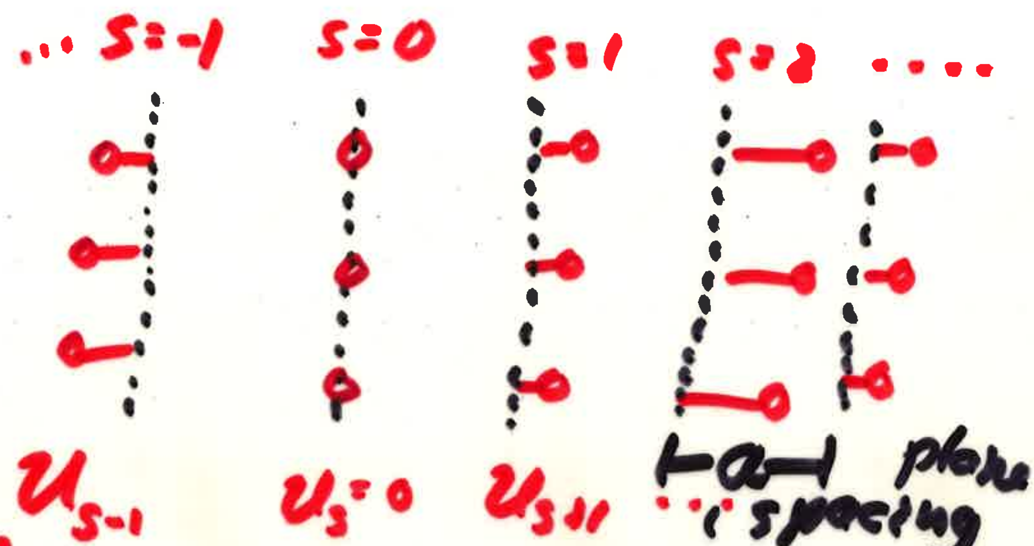
Phonons

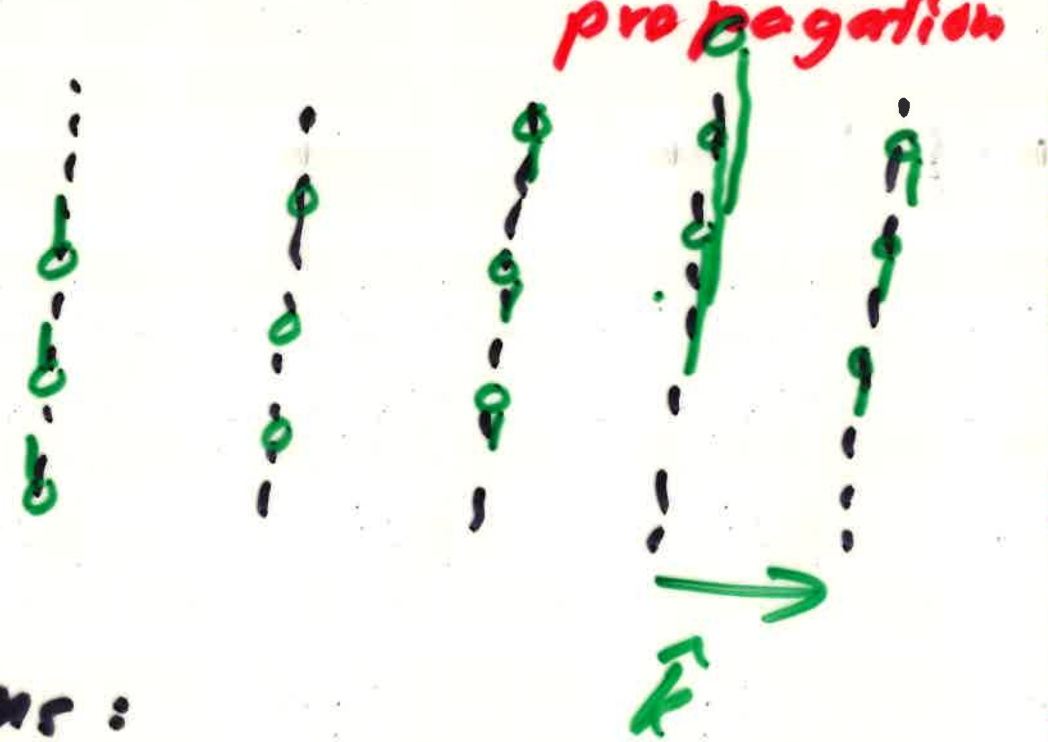
Longitudinal wave



displacements from equilibrium

$\hat{k}$ direction of energy propagation

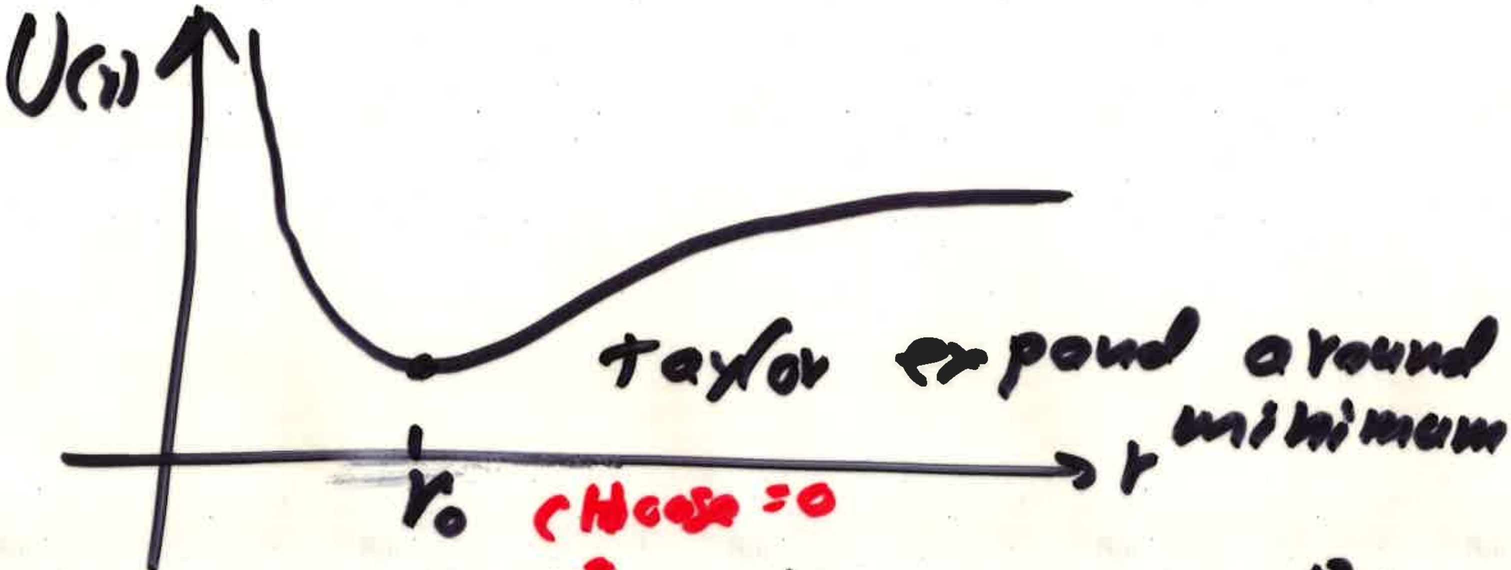
Transverse wave



Assumptions:

- nearest neighbor interaction <u>only</u>.
- force on a given atom is proportional to the displacement. Hooke's law.

Generic Potential



choose = 0

$$U(r) = \cancel{U_0} + \cancel{\frac{dU}{dr}}(r-r_0) + \frac{1}{2!}\frac{d^2U}{dr^2}\cdot(r-r_0)^2$$

$\rightarrow 0$ at minimum

$$= C\,u^2 + \cdots$$

↑ spring constant

Longitudinal waves

Force on an atom in the s-plane

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

$$M\frac{d^2u_s}{dt^2} = C\left[u_{s+1} - 2u_s + u_{s-1}\right]$$

Difference (not differential) equation.

Expect sinusoidal waves time dependence $e^{-i\omega t}$

$u_s \propto e^{-i\omega t}$ $\qquad \frac{d^2u_s}{dt^2} = -\omega^2 e^{-i\omega t}$

time part $\qquad = -\omega^2 u_s$

$$M \frac{d^2u_s}{dt^2} = C\left[u_{s-1} - 2u_s + u_{s+1}\right]$$

$$-M\omega^2 u_s = C\left[u_{s-1} - 2u_s + u_{s+1}\right]$$

space part

$$u_s = Ae^{ikx_s} = Ae^{ikas}$$

$$u_{s+1} = Ae^{ika(s+1)} = Ae^{ikas} \cdot e^{ika}$$

$$u_{s-1} = Ae^{ikas} \cdot e^{-ika}$$

$$-M\omega^2 A e^{ikas} = C e^{ikas} A \left[e^{-ika} - 2 + e^{ika} \right]$$

$$-M\omega^2 = C\left[2\cos(ka) - 2\right]$$

$$\omega^2 = \frac{2C}{M}\left[1 - \cos(ka)\right]$$

$$\omega^2 = \frac{4C}{M}\sin^2\left(\frac{ka}{2}\right)$$

$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Dispersion relation

Dispersion Relation $\omega(k)$

e.g. Light in vacuum

D.R. $\omega = c k$

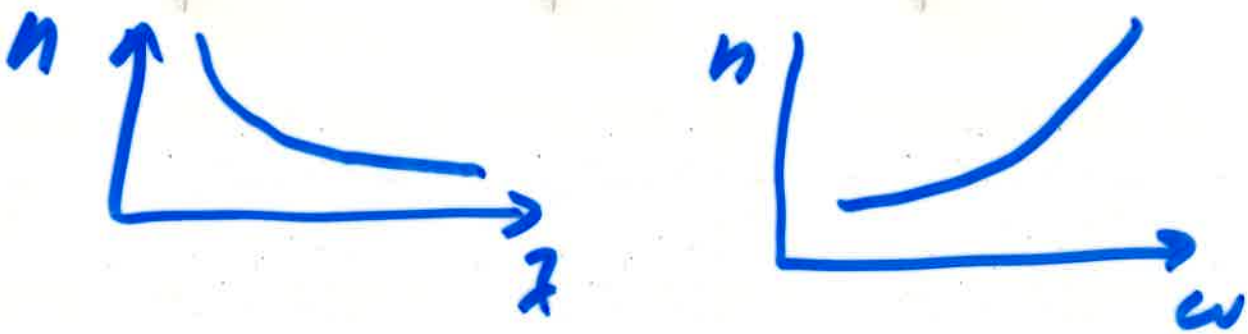
$\uparrow$ speed of light

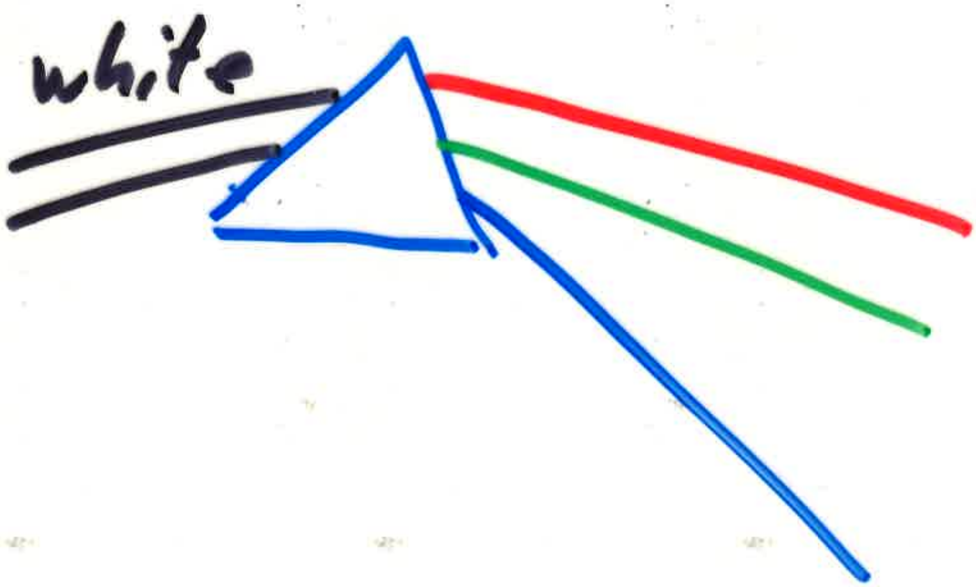
e.g. Light in a material with index of refraction $n(\omega)$

$n = 1$ vacuum

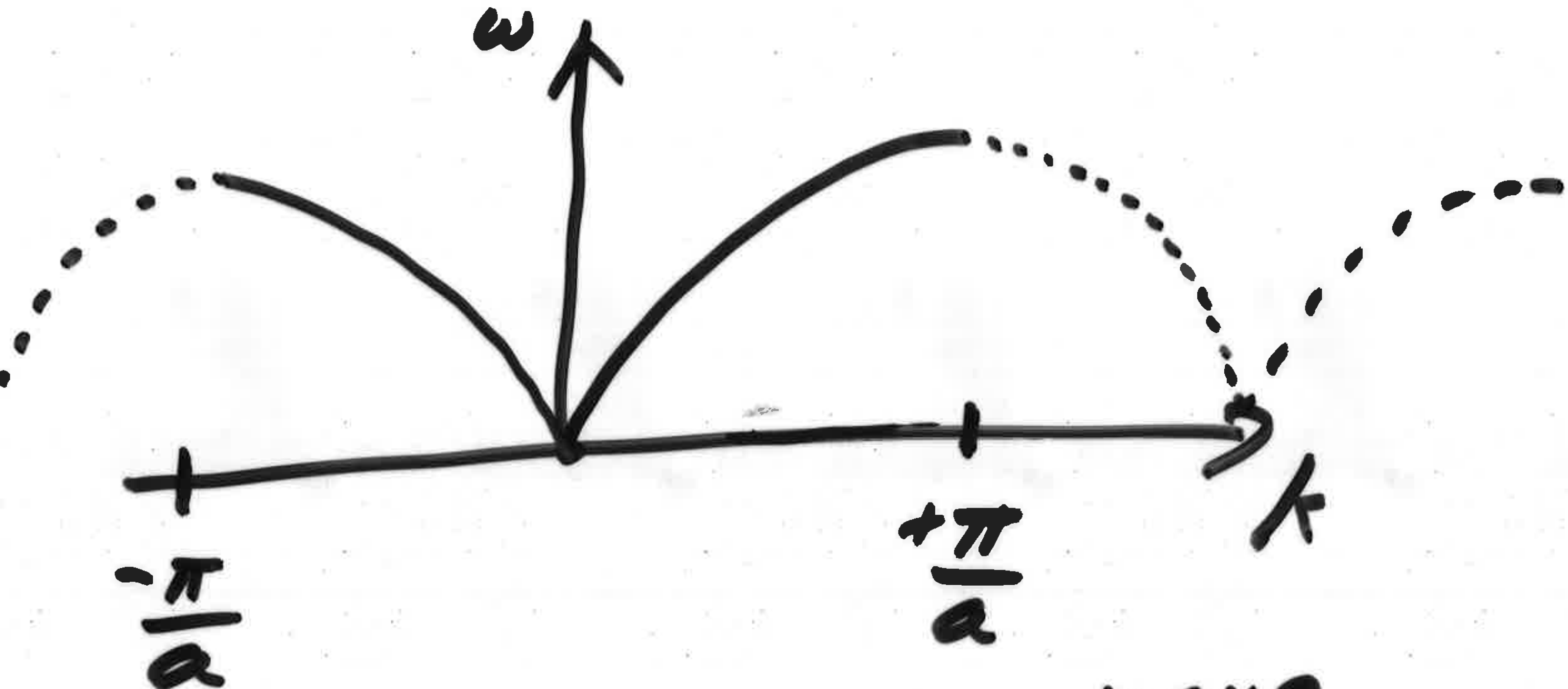
$n \geq 1$

D.R. $\omega = \dfrac{c}{n(\omega)} k$





D.R. $\omega = 2\sqrt{\frac{c}{M}}\,\left|\sin\left(\frac{ka}{2}\right)\right|$



Suppose we send a <u>wave packet</u> into the crystal

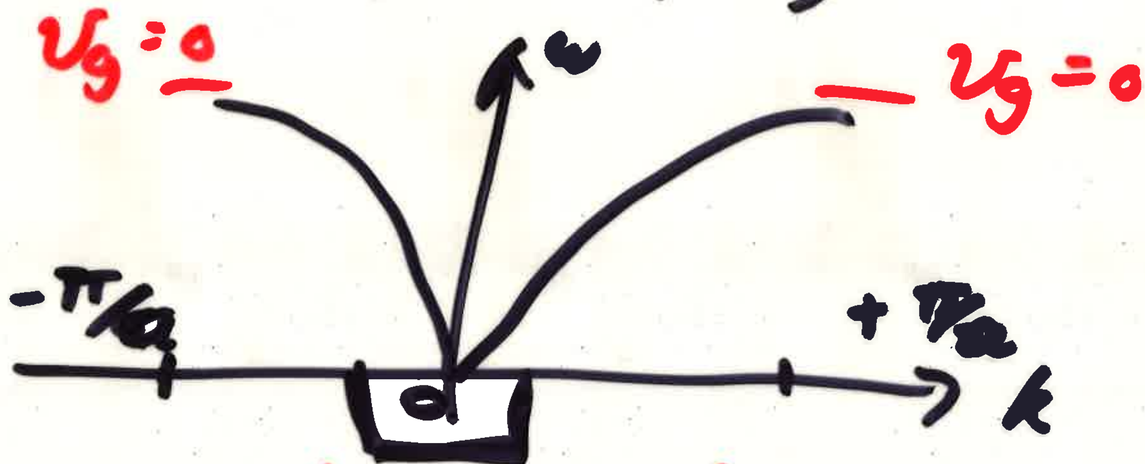
Two velocities

phase velocity $v_\varphi = \frac{\omega}{k}$

group velocity $v_g = \frac{d\omega}{dk}$

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left[2\sqrt{\frac{C}{m}}\sin\left(\frac{ka}{2}\right)\right]$$

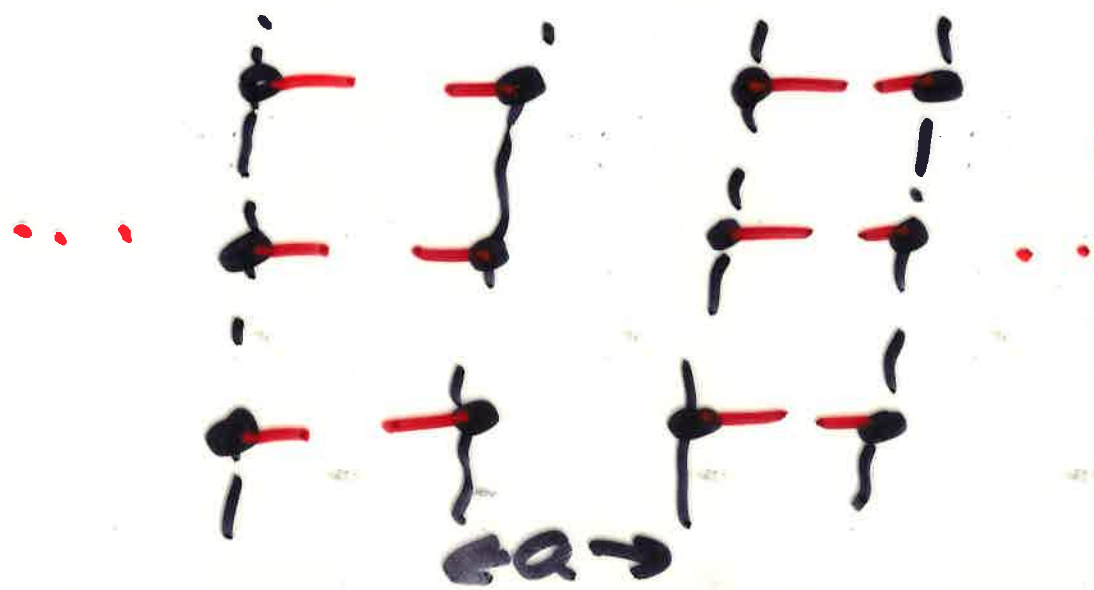
$$= a\sqrt{\frac{C}{M}}\cos\left(\frac{ka}{2}\right)$$



v_g is tangent slope

first Brillouin zone

At the zone boundaries $k = \pm\frac{\pi}{a}$



standing wave $v_g = 0$

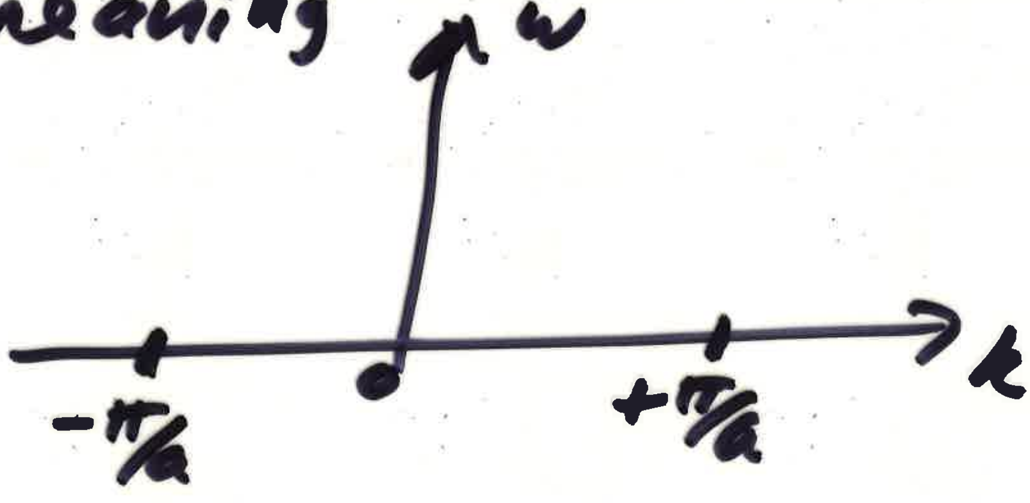
$$\frac{u_{s+1}}{u_s} = \frac{A e^{ika(s+1)}}{A e^{ikas}} = e^{ika}$$

At zone boundary $ka = \pm \pi$

$$\frac{u_{s+1}}{u_s} = e^{\pm i\pi} = -1$$

Only wavevectors k in the first Brillouin have physical meaning

$k = \frac{2\pi}{\lambda}$



$\lambda = a$

not allowed