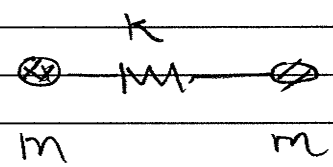
project:
P-1

Phonons

Having considered ~~static~~ crystal structures, let's consider vibrations. Begin with reminder of diatomic molecule.

We will focus on $d=1$ in all our discussion, because this already illustrates the key concepts



$$\left.\begin{aligned} m\ddot{x}_1 &= -k(x_1-x_2) \\ m\ddot{x}_2 &= -k(x_2-x_1) \end{aligned}\right\} \text{Newton's third law } F_{12} = -F_{21}$$

"Noether's Theorem" symmetry $\rightarrow$ conservation law

(could also do $m_1 \neq m_2$)

$$m(\ddot{x}_1 + \ddot{x}_2) = 0$$

$$\dot{x}_1 + \dot{x}_2 = \text{constant} = v_{cm}$$

$$(x_1 + x_2) = x_{cm}^0 + v_{cm}t$$

$$m(\ddot{x}_1 - \ddot{x}_2) = -2k(x_1-x_2)$$

$$\ddot{x}_1 - \ddot{x}_2 = -\frac{2k}{m}(x_1-x_2)$$ "relative coordinate"

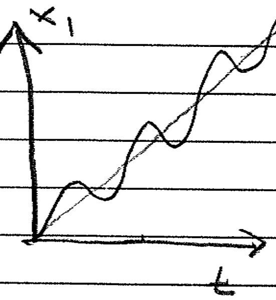
project:
P2

$$\begin{cases} x_1 - x_2 = A\cos\omega t + B\sin\omega t \\ x_1 + x_2 = x^{0}_{cm} + v_{cm}\, t \end{cases} \qquad \omega^2 = \frac{2k}{m}$$

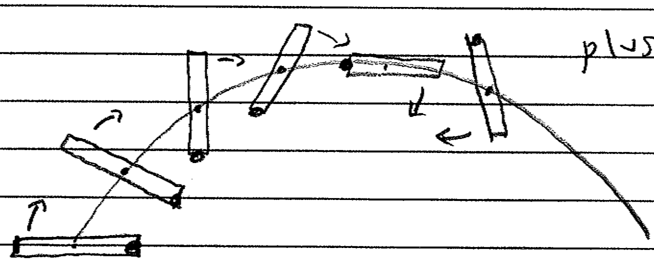
can get $x_1(t)$ $x_2(t)$ from these but perhaps simplest to think of motion decomposed in this way: CM moves at constant v

then ~~osc~~ oscillation about cm

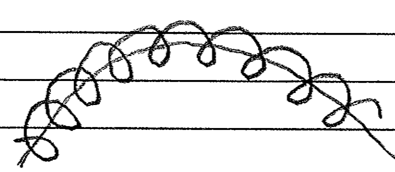
A, B, x^{0}_{cm}, v_{cm} from initial conditions $x^{0}_{1}, x^{0}_{2}, v^{0}_{1}, v^{0}_{2}$



Another example of "decomposed" motion (CM + angular) is thrown eraser. Suppose I asked you to describe $x(t), y(t)$ for tip of thrown eraser:



If rotation is <u>fast</u>:



project:

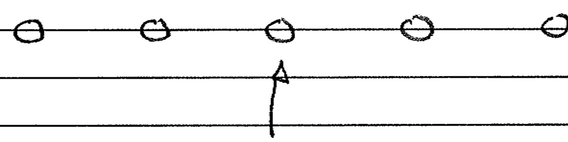
P3 Normal Mode frequencies $\omega^2 = 0$

$\omega^2 = 2k/m$

"Noether Theorem"

(translational) symmetry $\Rightarrow$ zero frequency mode

Many masses/springs (in 1d)



$$m\ddot{x}_n = -k(x_n - x_{n-1}) - k(x_{n+1} - x_n)$$

guess soln $x_n = a_n e^{i\omega t}$ (all $x_n(t)$ have same ω)

$$-m\omega^2 a_n = -k(a_n - a_{n-1}) - k(a_{n+1} - a_n)$$

Differential Eqns become algebraic Eqns

$$\begin{bmatrix} \ddots & & & & \\ -k & 2k & -k & & \\ & -k & 2k & -k & \\ & & -k & 2k & -k \\ & & & & \ddots \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = -m\omega^2 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

This looks like... an eigenvalue problem

project:

P4

Guess soln $a_n = a_0 e^{iqn}$

$\longrightarrow$ $-m\omega^2 e^{iqn} = -2k e^{iqn} + k e^{iq(n-1)} + k e^{iq(n+1)}$

a_0 cancels out

$$-m\omega^2 = -2k + k(\underbrace{e^{-iq} + e^{+iq}}_{2\cos q})$$

$$m\omega^2 = 2k - 2k\cos q$$

$$\omega^2 = \frac{2k}{m}\left[1 - \cos q\right]$$

$\boxed{\leftarrow P4!}$

1) N atoms but we got ∞ # of eigenvalues ?!

N dim matrix

2) Recover N=2 case how? Sort of resembles

N=2 in sense that $2k/m = \omega^2$ appears..

DiVOGA

project:
P4'

$$\omega^2 = \frac{2k}{m}\left[1-\cos q\right]$$

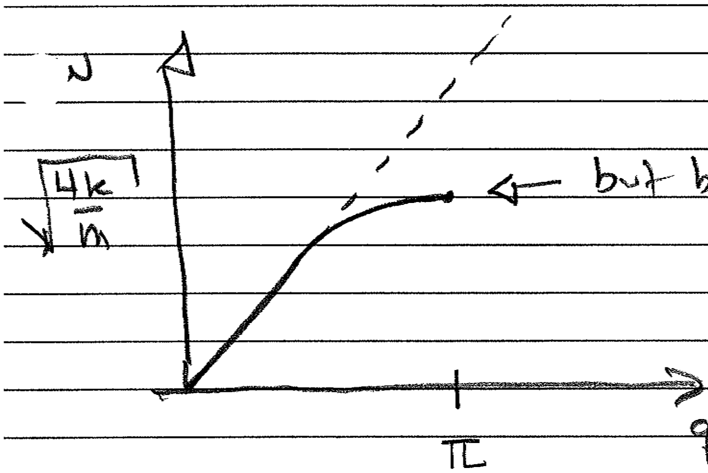
small q $\cos q \approx 1 - q^2/2$

$$\omega^2 = \frac{2k}{m}\, q^2/2 = k q^2/m$$

$$\omega = \sqrt{\frac{k}{m}}\, q$$ linear relation between ω and q

like photons

Hence name, phonons



← but bends over as q gets large

$\sqrt{\frac{k}{m}}\, a$ ← lattice constant

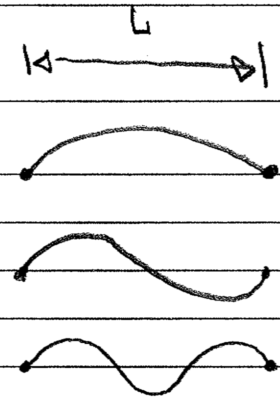
$\sqrt{\frac{k}{m}} = ??$ speed of sound in crystal

~ 300 m/s

DiVOGA

project:

P5



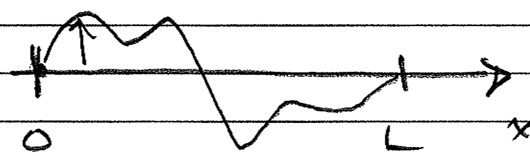
Analogy: vibrating string

not any λ will do:

needs to fit length of string $\lambda/2 = L$

$\lambda = L$

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



Boundary conditions

$y(x=0,t)=0$

$y(x=L,t)=0$

Review wave Eqn $\frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2}$ ↓ SKIP?!

$y(xt) = y = A(x)B(t)$ separation of variables

$AB'' = v^2 A'' B$ $\frac{B''}{B} = v^2 \frac{A''}{A} = -\omega^2$

constant

$\therefore B(t) \sim e^{\pm i\omega t}$

$\therefore A(x) \sim e^{\pm i\omega/v\, x}$ $k = \omega/v$ $\omega = vk$

$y(x,t) = \int c(k) e^{i(kx-\omega t)} + d(k) e^{i(kx+\omega t)} dk$

moves to right moves to left

project:

P6

or, if do not like complex exponentials

$y(x\,t) =$ $\sin kx \sin \omega t$; $\sin kx \cos \omega t$;

$\cos kx \sin \omega t$; $\cos kx \cos \omega t$;

suppose we want $y(x=0, t) = 0 \quad \forall t$

insist on no $\cos kx$ terms

$y(x\,t) = \sin kx \sin \omega t \quad \sin kx \cos \omega t$

if $y(x=L, t) = 0 \quad \forall t$ also then $k = \frac{\pi}{L} n$

$$y(x,t) = \sum_n \left[c_n \sin \frac{n\pi}{L} x \cos \frac{n\pi v}{L} t + d_n \sin \frac{n\pi x}{L} \sin \frac{n\pi v}{L} t \right]$$

How are c_n and d_n determined?!

$y(x,0)$

and Fourier series stuff

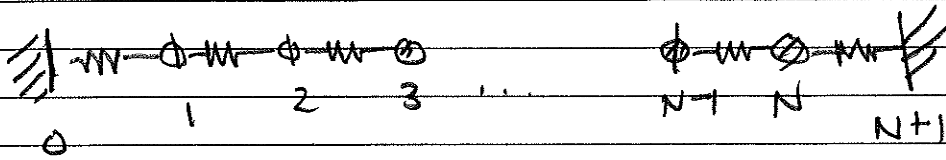
$dy/dt\,(x,0)$

Skip!?

project:

P7

① Boundary conditions $X_0 = X_{N+1} = 0$ connect to wall



$$\cancel{m}\ddot{x}_1 = -k(x_1 - \phi) - k(x_1 - x_2)$$

② free end $\ddot{x}_1 = \boxed{\cancel{}} \; - k(x_1 - x_2)$

missing neighbor.

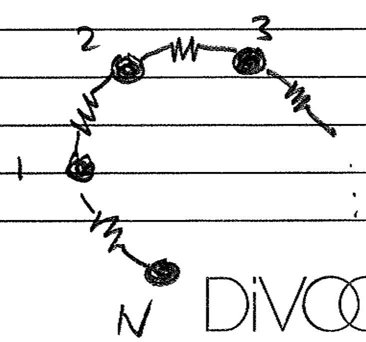
③ "periodic bdy conditions"

① and ② are mathematically more difficult.

Instead

$$\ddot{x}_1 = \boxed{-k(x_1 - x_N)} - k(x_1 - x_2)$$
$$\ddot{x}_N = -k(x_N - x_{N-1}) \boxed{-k(x_N - x_1)}$$

Why might this be "better" ?! ③ is more symmetric! masses 1, N have 2 moving neighbors like all the rest. There are no "ends" which are "special"



project:

P8

Implementation:

In original eqns

$$m\ddot{x}_n = -k(x_n - x_{n-1}) - k(x_n - x_{n+1})$$

Identity $\quad x_{N+1} \equiv x_1$

$$x_0 \equiv x_N$$

In matrix:

k

$$\begin{bmatrix} 2k & -k & & & & \boxed{} \\ -k & 2k & -k & & & \\ & -k & 2k & -k & & \\ & & & & & \\ & & & & & \\ \boxed{} & & & & -k & 2k \end{bmatrix} \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ \vdots \\ \\ q_N \end{pmatrix}$$

k

$$x_{N+1} = x_1 \Rightarrow q_{N+1} = q_1 \Rightarrow e^{iqN} = 1$$
$$x_0 \equiv x_N \qquad q_0 = q_N$$

$$q \;\cancel{\ }\; = \frac{2\pi}{N}\{0, 1, 2, \ldots N-1\}$$

← N dim matrix now has N eigenvalues as expected

DiVOGA

project:
P9

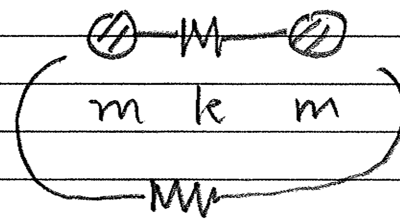
Recover $N = 2$ case $\omega = 0$

$$\omega = \sqrt{\frac{2k}{m}}$$

$N = 2$ $\quad q = \frac{2\pi}{2}\{0,1\} = 0, \pi$

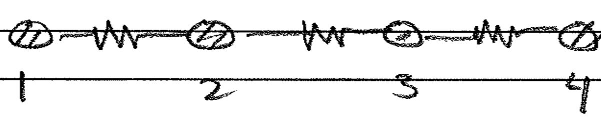
$$\omega^2 = \frac{2k}{m}\left[1 - \cos q\right] = 0, \frac{4k}{m}$$

Looks a bit different!
why?



PBC gives extra
spring k between $1, N$
$N=2$ case k is doubled

Normal modes of 4 masses



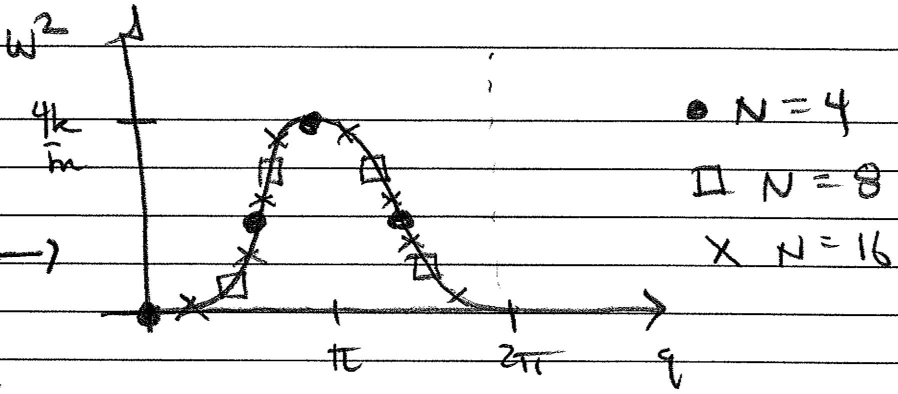
$$\omega^2 = \frac{2k}{m}\left[1 - \cos q\right] = 0, \frac{2k}{m}, \frac{4k}{m}, \frac{2k}{m}$$

$$q = \frac{2\pi}{4}\{0,1,2,3\}$$

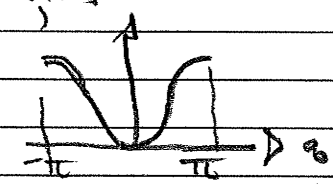
project:

P10

Pictorially



Actually usually allow $q \in [-\pi, \pi]$ →



Now do case of 2 different atoms, masses M_1 M_2

n odd $\qquad M_1 \ddot{x}_n = -k(x_n - x_{n+1}) - k(x_n - x_{n-1})$

n even $\qquad M_2 \ddot{x}_n = -k(x_n - x_{n+1}) - k(x_n - x_{n-1})$

again assume all x_n (odd and even) have same ω

$$x_n(t) = \begin{cases} a_n e^{i\omega t} & n \text{ odd} \\ b_n e^{i\omega t} & n \text{ even} \end{cases}$$

but let amplitudes be different for odd, even

$$a_n = a_0 e^{iqn}$$
$$b_n = b_0 e^{iqn}$$

like same ω: same q
just different amplitude

project:
P11

Two eqns result

n odd $\quad -M_1 w^2 a_0 = -k(a_0 - b_0 e^{iq}) - k(a_0 - b_0 e^{-iq})$

n even $\quad -M_2 w^2 b_0 = -k(b_0 - a_0 e^{iq}) - k(b_0 - a_0 e^{-iq})$

$$\begin{pmatrix} 2k - M_1 w^2 & -2k\cos q \\ -2k\cos q & 2k - M_2 w^2 \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

what must happen?? need $| \, | = 0$

$$(2k - M_1 w^2)(2k - M_2 w^2) - 4k^2\cos^2 q = 0$$

$$M_1 M_2 w^4 - 2k(M_1+M_2) w^2 + 4k^2(1-\cos^2 q) = 0$$

$\boxed{\text{P11'' FIRST}} \rightarrow$ $\quad 2\sin^2 q/2 \quad$ $1 = \cos^2\theta + \sin^2\theta$ $\quad \cos 2\theta = \cos^2\theta - \sin^2\theta$

$$w^2 = \frac{1}{2M_1M_2}\left[2k(M_1+M_2) \pm \sqrt{4k^2(M_1+M_2)^2 - 4M_1M_2 4k^2 \sin^2\frac{q}{2}}\right]$$

... DO NOT COMPLETE ...

General comments on strategy:

Normal Modes $\leftrightarrow$ diagonalize matrix

kspace often does it, or almost does it (leftover 2x2 matrix)

DiVOGA

project:

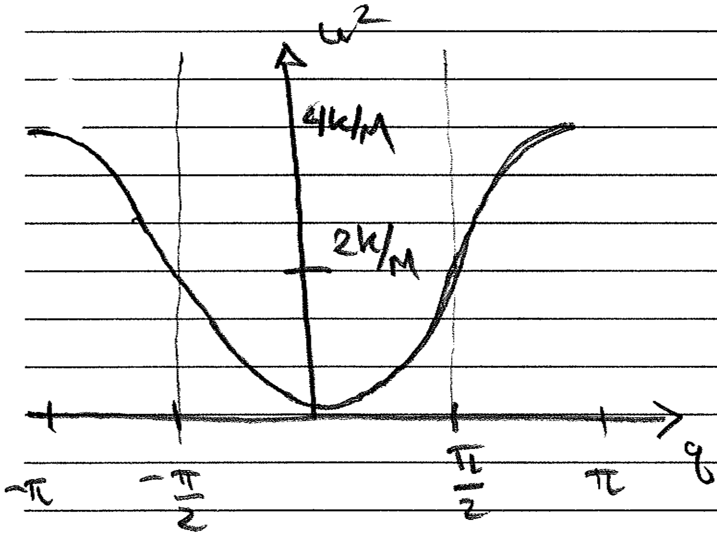
P 11'

Counting?

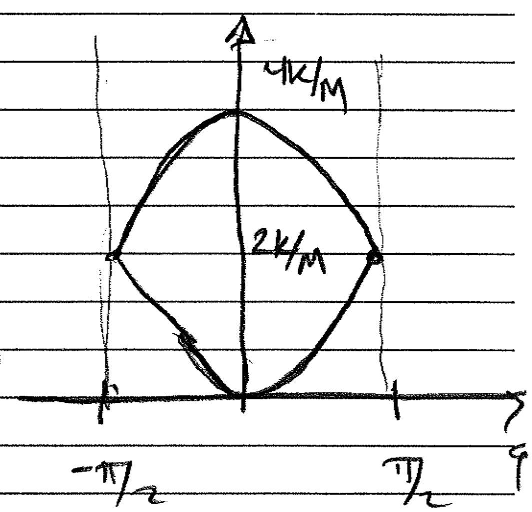
We want N eigenvalues, but for each q we seem to have 2 ω^2 values. If there are still N q values we would have $2N$ eigenvalues?!

Instead q is now restricted to $(-\pi/2, \pi/2)$ (1/2 allowed values). One way to see is that repeated unit is pair of atoms

M_1 — M_2

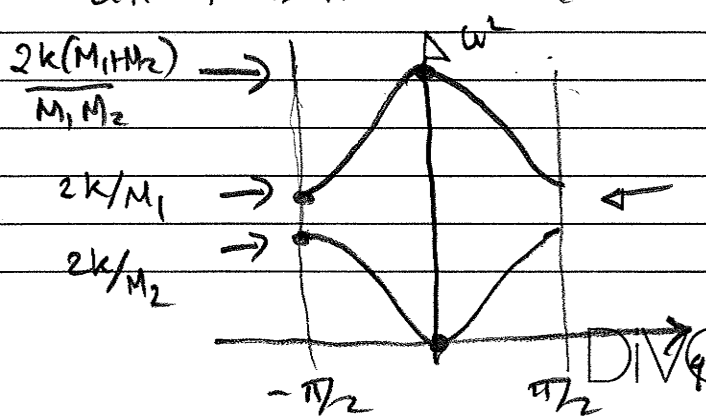


$\leftarrow$ $M_1 = M_2$ case can also be viewed with "folded" zone $\rightarrow$



(same exact set of ω^2)

allows better connection to $M_1 \neq M_2$ case where $q \in (-\frac{\pi}{2}, \frac{\pi}{2})$



key point is gap opens in spectrum.

(same math in e^- moving on lattice of nuclei $\rightarrow$ "band insulators")

project:

P11''

Do limiting cases first : $q = 0 \qquad \cos q = 1$

$$(2k - M_1 w^2)(2k - M_2 w^2) - 4k^2 = 0$$

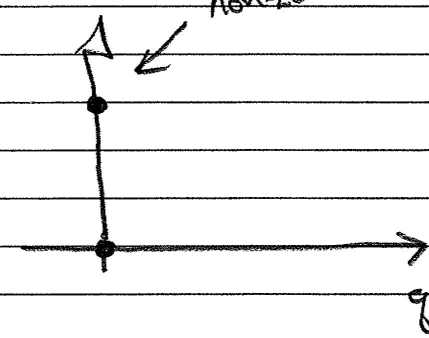
$$M_1 M_2 w^4 - 2k(M_1 + M_2) w^2 = 0$$

$$w^2 \left(w^2 M_1 M_2 - 2k(M_1 + M_2) \right) = 0$$

nonzero @ $q=0$!

1) $w^2 = 0$

2) $w^2 = \dfrac{2k(M_1 + M_2)}{M_1 M_2}$



$q = \pi/2 \qquad \cos q = 0$

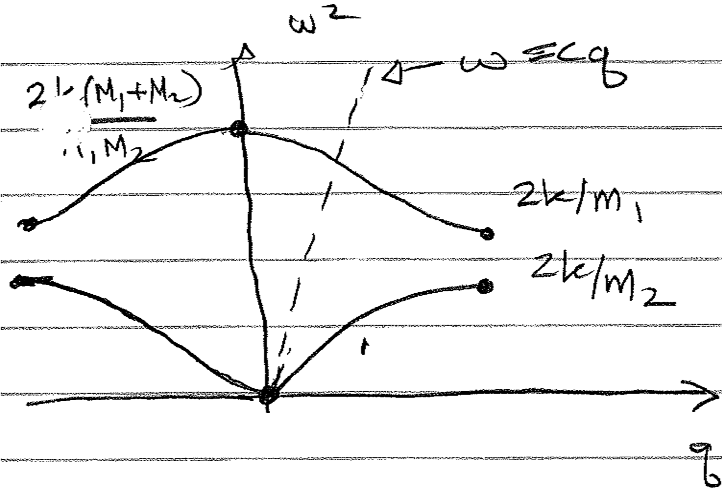
$$M_1 M_2 w^4 - 2k(M_1 + M_2) w^2 + 4k^2 = 0$$

$$w^2 = \frac{1}{2 M_1 M_2} \left[2k(M_1 + M_2) \pm \sqrt{4k^2 (M_1 + M_2)^2 - 16 M_1 M_2 k^2} \right]$$

$$\pm \sqrt{4k^2 (M_1 - M_2)^2}$$

$$w^2 = \frac{1}{2 M_1 M_2} \left[2k(M_1 + M_2) \pm 2k(M_1 - M_2) \right]$$

$$w = \frac{K}{M_1 M_2} \left[M_1 + M_2 \pm (M_1 - M_2) \right] \quad \xrightarrow{+} 2k/M_2 \qquad \xrightarrow{-} 2k/M_1$$



lower branch: "acoustic phonons" $\omega = vq$ as before

upper branch: "optical phonons"

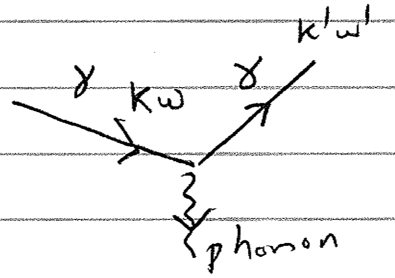
these phonons get excited when light passes through solid

$\omega = cq$

General principle: different excitations couple

if there dispersion relations intersect/overlap

Reason: Energy and momentum match up



for acoustic phonons if photon γ needs to transfer ~~energy ω~~ momentum $k - k'$ the associated energy $\omega - \omega' \sim c(k - k')$ is likely to be way more than acoustic phonon can accomodate.

What changes in 3D? Very little.

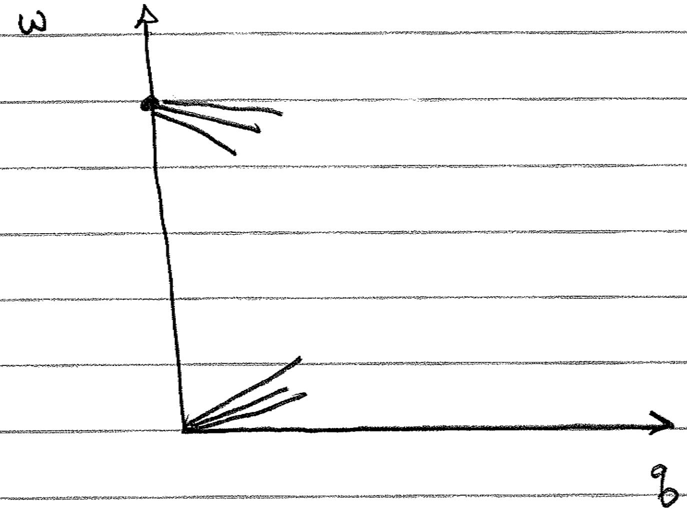
Basically 2 modes

optic / acoustic → 6 modes

(3 optic ; 3 acoustic)

because atoms can vibrate in 3 directions

$x \to x, y, z$



Often label modes Longitudinal vs transverse according to whether displacement is $\parallel$ or $\perp$ to propagation direction

bulk vs shear modulus → building properties steel girders vs concrete pillars

$\left\{\begin{array}{l} \text{vibrating string} \leftarrow \text{transverse} \\ \text{sound in pipe (compression wave)} \leftarrow \text{longitudinal} \end{array}\right.$

light ← $\vec{E}, \vec{B}$ oscillations $\parallel$ or $\perp$ to $\vec{k}$?

$$\vec{E}(\vec{r}) = \vec{E}_0 e^{i\vec{k}\cdot\vec{r}} \qquad \vec{\nabla}\cdot\vec{E} = 0$$

earthquakes ?