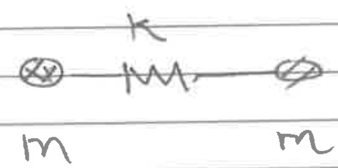
project:
P-1

$\boxed{\text{Phonons}}$

Having considered <u>static</u> 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



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

"Noether's Theorem" symmetry → conservation law

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

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

(could also do $m_1 \neq m_2$)

$$(x_1 + x_2) = x^0_{cm} + V_{cm}\, t$$

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

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

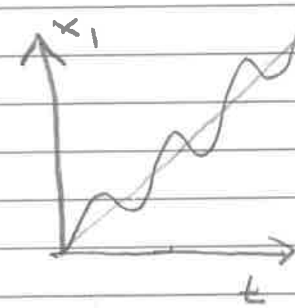
project:

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

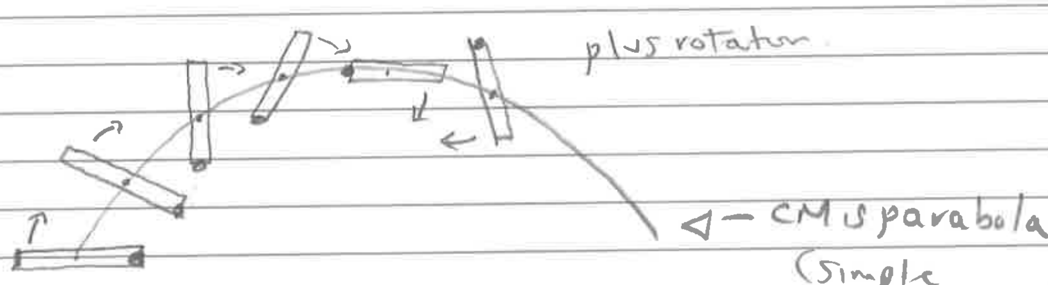
then ~~over~~ oscillation about cm



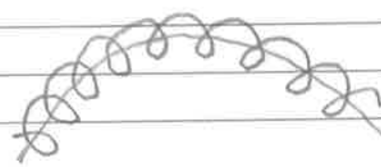
A, B, x^0_{cm}, v_{cm} from initial conditions

$x^0_1, x^0_2, v^0_1, v^0_2$

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 fast:



project:

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

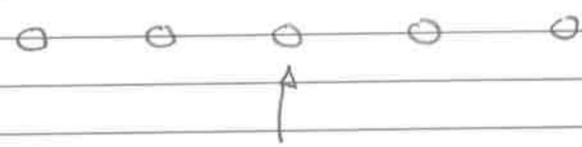
$\omega^2 = 2k/m$

"Noether Theorem"

~~[illegible]~~"

(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 $a_n = a_0 e^{iqn}$

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

a_0 cancels out

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

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

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

$\boxed{\Leftarrow \text{P4!}}$

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..

project:
P4'

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

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

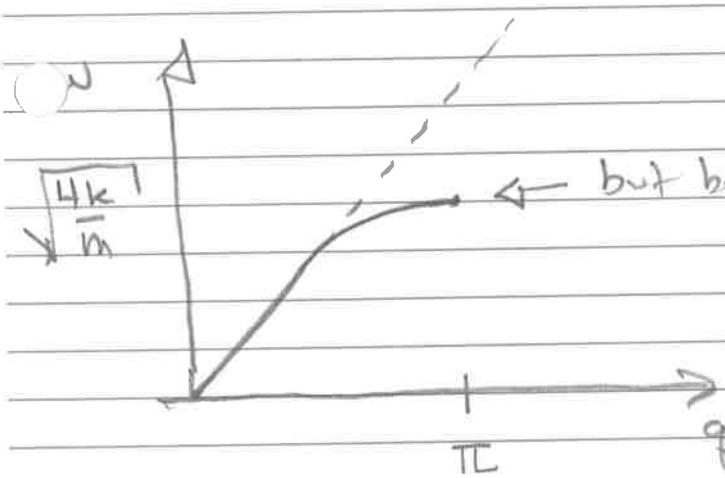
$$\omega^2 = \frac{2k}{m}\, q^2/2 = kq^2/m$$

$$\omega = \sqrt{\frac{k}{m}}\, q$$

linear relation between ω and q

like photons

Hence name, phonons

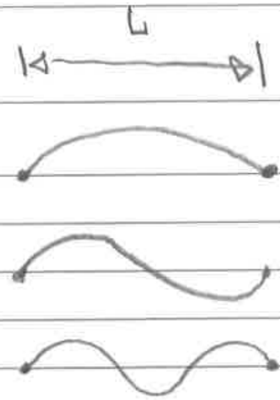


$\sqrt{\frac{k}{m}}\, a$ lattice constant

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

~ 300 m/s

project:
P5



Analogy: vibratory string

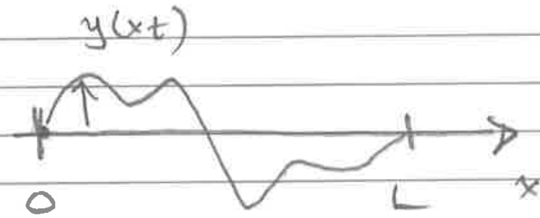
not any λ will do:

needs to fit length of

string $\lambda/2 = L$

$\lambda = L$

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



Boundary conditions

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

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

Skip?!

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

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

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

constant

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

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

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

moves to Right $\qquad$ 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 $k = \frac{\pi}{L} n$

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

How are c_n and d_n determined ?!

$y(x,0)$

and Fourier series stuff

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

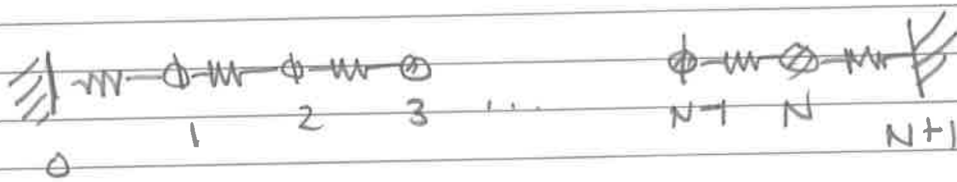
↑ Skip !?

DiVOGA

project:

P7

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



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

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

missing neighbour.

③ "periodic bdy conditions"

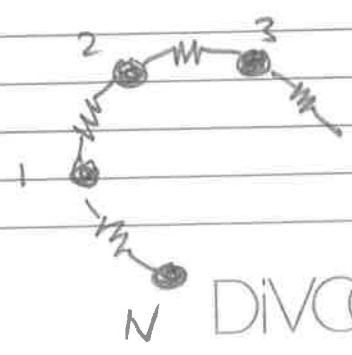
① and ② are mathematically more difficult.

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 $x_{N+1} \equiv x_1$

$$x_0 \equiv x_N$$

In matrix:

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

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

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

N dim matrix now has N eigenvalues as expected

DIVOGA

project: P9

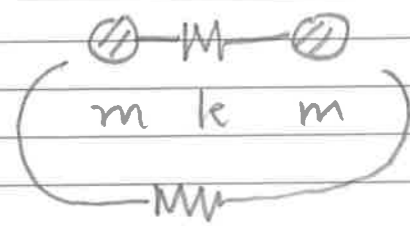
Recover $N = 2$ case $\omega = 0$

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

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

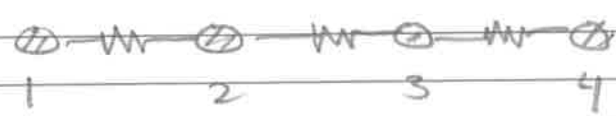
$$\omega^2 = \frac{2k}{m}\left[1 - \cos q\right] = 0, \frac{4k}{m}$$

Looks a bit different!
why?



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

Normal modes of 4 masses

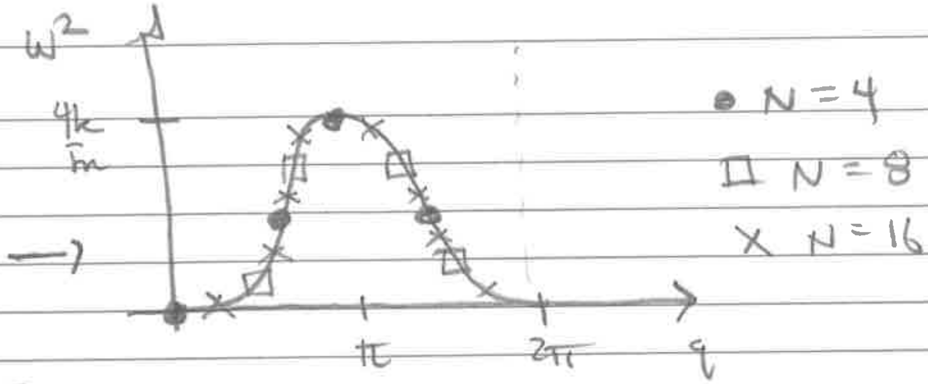


$$\omega^2 = \frac{2k}{m}\left[1 - \cos q\right] = 0, \frac{2k}{m}, \frac{4k}{m}, \frac{2k}{m}$$

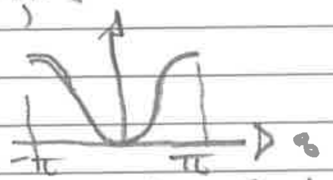
$$q = \frac{2\pi}{4}\{0, 1, 2, 3\}$$

project: P10

Pictorially



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



Now do case of 2 different atoms, masses M_1 M_2

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

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

again assume <u>all</u> x_n (odd <u>and</u> 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 $| \; | = 0$

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

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

$\boxed{\text{“P11” FIRST}} \longrightarrow$ $\quad 2\sin^2 q/2$

$1 = \cos^2\theta + \sin^2\theta$

$\cos 2\theta = \cos^2\theta - \sin^2\theta$

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

... DO NOT COMPLETE ...

General comments on strategy:

Normal Modes $\leftrightarrow$ diagonalize matrix

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

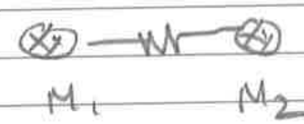
project:

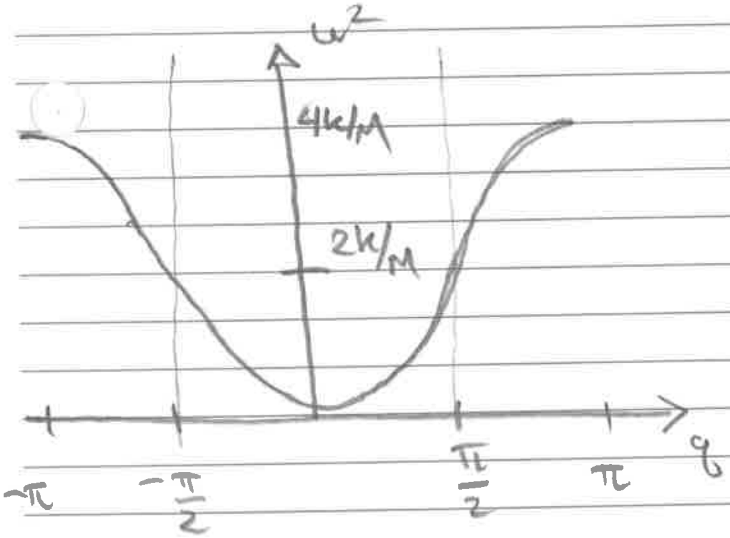
P 11'

Counting ?

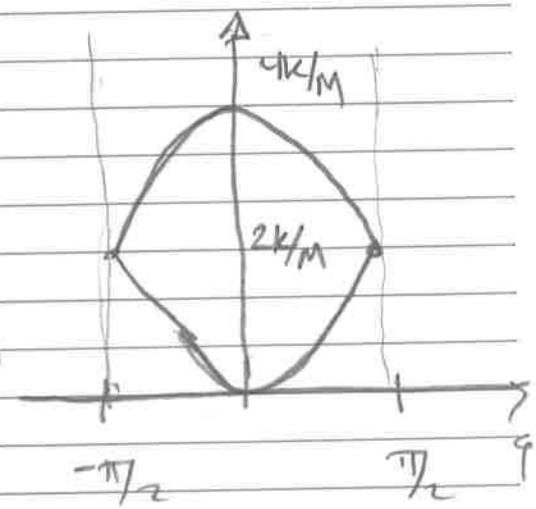
We want N eigenvalues, but for each q we seem to have 2 ω^2 values. If there are still N q values we would have $2N$ eigenvalues ?!

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



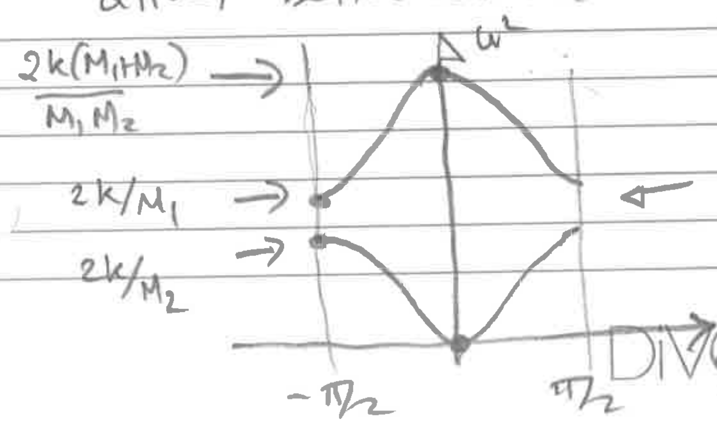


← $M_1 = M_2$ case can also be viewed with "folded" zone →



(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 → "band insulators")

project:

P11''

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

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

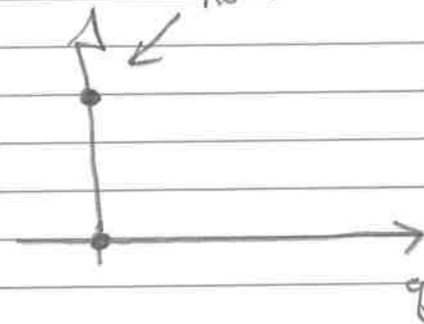
$$M_1 M_2 w^4 - 2k(M_1+M_2)w^2 = 0$$

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

nonzero @ $q=0$!

1) $w^2 = 0$

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



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

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

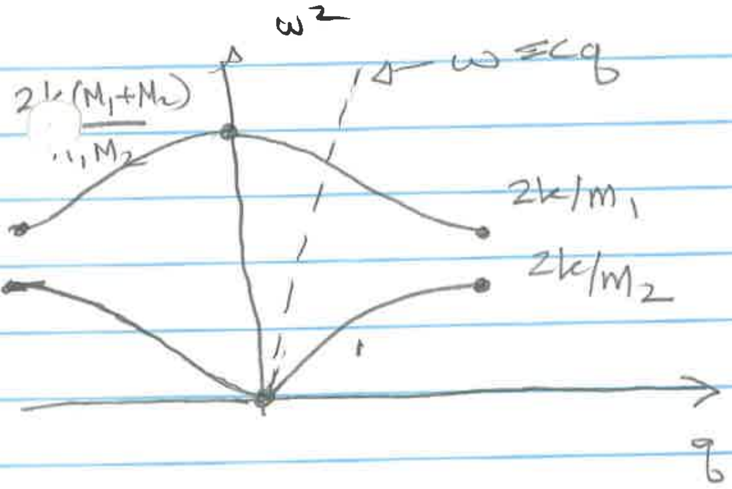
$$w^2 = \frac{1}{2M_1M_2}\left[2k(M_1+M_2) \pm \sqrt{4k^2(M_1+M_2)^2 - 16 M_1 M_2 k^2}\right]$$

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

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

$$w = \frac{K}{M_1M_2}\left[M_1+M_2 \pm (M_1-M_2)\right] \begin{array}{l} \xrightarrow{+} 2k/M_2 \\ \xrightarrow{-} 2k/M_1 \end{array}$$

p12



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

upper branch : "optical phonons"

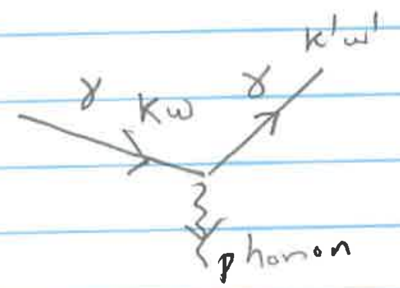
these phonons get excited when light passes through solid

$\omega = cq$

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~~
momentum $k - k'$ the
associated energy $\omega - \omega' \sim c(k-k')$
is likely to be way more than
acoustic phonon can accommodate.

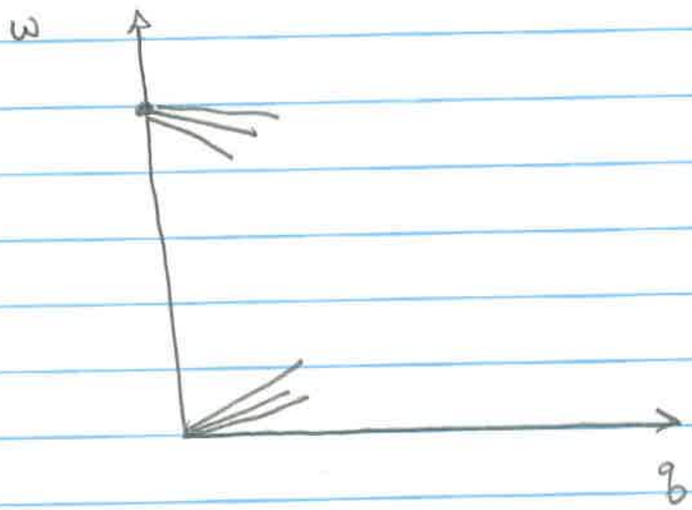
p13.

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

vibrating string ← transverse

sound in pipe (compression wave) ← longitudinal

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

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

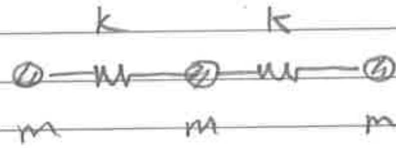
$\vec{E}(\vec{r}) = \vec{E}_0 e^{i\vec{k}\cdot\vec{r}}$ $\vec{\nabla}\cdot\vec{E} = 0$

earthquakes ?

project: 1

Connections of Normal Mode of N mass/spring to other problems.

Triatomic molecule:



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

$$m\ddot{x}_2 = -k(x_2 - x_1) - (x_2 - x_3) \qquad x_n(t) = a_n e^{i\omega t}$$

$$m\ddot{x}_3 = -k(x_3 - x_2)$$

$$\frac{k}{m}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \omega^2 \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$$

$$\vec{V}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad \omega^2 = 0$$

$$\vec{V}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \qquad \omega^2 = \frac{k}{m}$$

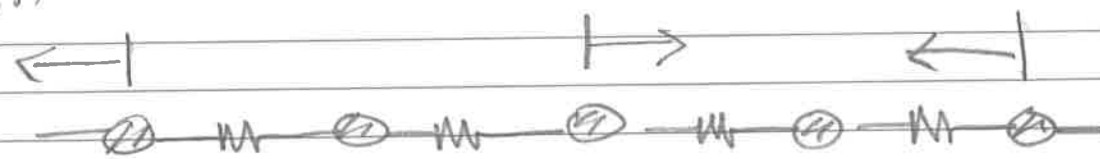
← Similar to HW problem central mass doesn't move

$$\vec{V}_3 = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \qquad \omega^2 = \frac{3k}{m}$$

project:

(2)

HW problem points out some interesting modes of M_1, M_2 system



M_2 at rest : obviously $\omega^2 = 2k/m_1$

likewise M_1 at rest.

These come out of our general soln.

In fact they are part of $M_1 = M_2$ case

$$\frac{k}{m}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \cdots & -1 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ & & & & & & \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \omega^2 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}$$

Before we discussed $\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \vdots \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ \vdots \end{pmatrix}$

e^{iqn} $q=0$ $\qquad$ e^{iqn} $q=\pi$

But notice $\begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \end{pmatrix}$

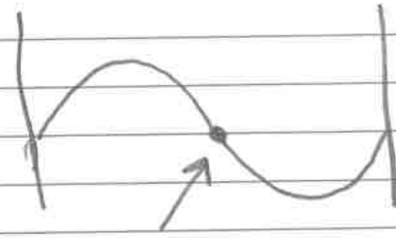
e^{iqn} $\rightarrow$

$q=\pi/2$ and $-\pi/2$ Δ - degenerate $\quad \cos qn \quad q=\pi/2$

project:
③

More connections!

* Vibrating strings have nodes



Analogy is this mode
has same ω^2 when $M_2 \neq M_1$
since M_2 never moves

If you put a little massive
bead here
ω^2 unchanged!

* In QM class ∞ square well
perturbation of $V\delta(x-a)$
if a is at node of ϕ_n^0 ← eigenstate of H^0
then $E_n^1 = 0$ no energy shift.

Time indep Sch Eqn

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x\,t)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V(x)\psi(x)=E\psi(x)$$

Laplace/Poisson Eqn

$$E=-\nabla\phi$$

$$\nabla\cdot E=\rho/\epsilon_0$$

$$-\nabla^2\phi(x)=\rho(x)/\epsilon_0$$

Diffusion Eqn

$$\frac{\partial\rho(x\,t)}{\partial t}=k\nabla^2\rho(x\,t)$$

So ∇^2 ubiquitous QM, EM, CM

$$\frac{df}{dx}=\frac{f(x+\Delta x)-f(x)}{\Delta x}$$

$$\frac{d^2f}{dx^2}=\frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{(\Delta x)^2}$$

$$\frac{d^2f}{dx^2}\rightarrow -1\begin{bmatrix} -1 & +2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \end{bmatrix}\begin{bmatrix} f((n-1)\Delta x) \\ f(n\Delta x) \\ f((n+1)\Delta x) \end{bmatrix}$$