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

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

$$
\begin{align*}
-\frac{k}{m} \Delta x(y) &= -k(x_1 - x_2) \\
\Delta x(\infty) &= -k(x_2 - x_1)
\end{align*}
$$

Newman's principle: $F_{12} = -F_{21}$

$$m \Delta \ddot{x} = 0$$

Noether's theorem: symmetry $\Rightarrow$ conservation law

$\Delta x_1 + \Delta x_2 = 0$ (could also $\Delta x_1 = \Delta x_2$)

$\Delta x_1 + \Delta x_2 = \text{constant} = v_{cm}$

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

$$m(x_1 - x_2) = -2k(x_1 - x_2)$$

$$\frac{x_1 - x_2}{x_1^0 - x_2^0} = \frac{-2k}{m} (x_1 - x_2) \quad \text{"relative coordinate"}$$
\[ x_1 - x_2 = A \cos \omega t + B \sin \omega t \]
\[ x_1 + x_2 = x^0_{cm} + V_{cm} t \]

Can get \( x_1(t), x_2(t) \) from here but perhaps simpler to think of motion decomposed in this way: CM moves at constant \( V \)

Then angular oscillation about CM.

\[ A, B, x^0_{cm}, V_{cm} \] from initial condition.

\[ x^0_1, x^0_2, V^0_1, V^0_2 \]

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.

\( \Delta - CM \) is parabola (single)

If rotation is fast...
Normal Mode frequencies $w^2 = 0$

$w^2 = 2k/m$

"Noether Theorem"

(Translated) 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 $x_n = q_n e^{iwt}$ (all $x_n(t)$ have same $w$)

\[ -mw^2q_n = -k(q_n - q_{n-1}) - k(q_{n+1} - q_n) \]

\[
\begin{bmatrix}
-k & 2k & -k \\
-k & 2k & -k \\
-k & 2k & -k
\end{bmatrix}
\begin{bmatrix}
q_1 \\
q_2 \\
q_3 \\
q_4
\end{bmatrix}
= -mw^2
\begin{bmatrix}
q_1 \\
q_2 \\
q_3 \\
q_4
\end{bmatrix}
\]

This looks like an eigenvalue problem

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Guess solution: \( a_n = a_0 e^{i \phi n} \)

\[-m \omega^2 e^{i \phi n} = -2k e^{i \phi n} + k e^{i \phi (n-1)} + k e^{i \phi (n+1)}\]

\(a_0\) cancels out:

\[-m \omega^2 = -2k + k(e^{-i \phi} + e^{i \phi})\]

\[2 \cos \phi\]

\[m \omega^2 = 2k - 2k \cos \phi\]

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

\[\boxed{\text{p41}}\]

1) \( N \) atoms but we got \( 2N \) # of eigenvalues?!

A \( N \times N \) matrix

2) Recover \( N=2 \) case from? Sort of resembles:

\( N=2 \) in sense that \( \frac{2k}{m} = \omega^2 \) appears...
\[ w^2 = \frac{2k}{m} [1 - \cos q] \]

Small \( q \), \( \cos q \approx 1 - \frac{q^2}{2} \)

\[ w^2 = \frac{2k}{m} \frac{q^2}{2} = \frac{kq^2}{m} \]

\[ w = \sqrt{\frac{k}{m}} q \quad \text{linear relation between } w \text{ and } q \]

Like photon

Hence name, phonons

\[ \sqrt{\frac{k}{m}} = \sqrt{\frac{\hbar^2}{m}} \quad \text{linear constant} \]

\[ \sqrt{\frac{k}{m}} = \frac{\hbar}{m} \quad \text{speed of sound in crystal} \]

\approx 300 \text{ m/s} \]

\[ \]
Analog: Vibratory string

not any \( \lambda \) 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:

\[ \frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2} \]

\[ y(x,t) = y = A(x) B(t) \] \( \Rightarrow \) Separation of Variables

\[ A B'' = \frac{\partial^2 A}{\partial x^2} B \]

\[ \frac{B''}{B} = -\frac{\partial^2 A}{A} = -\omega^2 \]

\[ B(t) \sim e^{\pm i\omega t} \]

\[ A(x) \sim e^{i\omega k x} \quad k = \frac{\omega}{v} \quad \omega = vk \]

\[ y(x,t) = \int c(k) e^{i(kx-wt)} + d(k) e^{i(kx+wt)} \quad dk \]

\[ \text{moves to right} \quad \text{moves to left} \]
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 \[ y(x=L, t) = 0 \quad \forall t \] then \[ k = \frac{n \pi}{L} \]

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

How are \( c_n \) and \( d_n \) determined?

\[ y(x,0) \quad \text{and Fourier series stuff} \]

\[ dy/dt (x,0) \]

\[ \text{Skip!} \]
Boundary conditions: $x_0 = x_{N+1} = 0$ (no wall).

\[
\begin{align*}
\dot{x}_1 &= -k(x_1 - x_0) - k(x_1 - x_2) \\
\dot{x}_i &= -k(x_i - x_{i-1}) - k(x_i - x_{i+1})
\end{align*}
\]

2) free end: $\dot{x}_1 = -k(x_1 - x_2)$

3) periodic boundary conditions:

1) and 2) are mathematically more difficult.

Instead:

\[
\begin{align*}
\dot{x}_1 &= -k(x_1 - x_N) - k(x_1 - x_2) \\
\dot{x}_N &= -k(x_N - x_{N-1}) - k(x_N - x_1)
\end{align*}
\]

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."
Implementation:

In original eqn:

\[ m x_n = -k(x_n - x_{n-1} - k(x_n - x_{n+1}) \]

Identity: \( x_{n+1} = x_1 \)

\( x_0 = x_N \)

In matrix:

\[
\begin{pmatrix}
2k & -k & & & \\
-k & 2k & -k & & \\
& -k & 2k & -k & \\
& & & \ddots & \ddots \\
& & & -k & 2k \\
\end{pmatrix}
\begin{pmatrix}
q_1 \\
q_2 \\
q_3 \\
\vdots \\
q_N \\
\end{pmatrix}
\]

\[ x_{n+1} = x_1 \Rightarrow q_{n+1} = q_1 \Rightarrow e^{i\beta N} \]

\[ x_0 = x_N \Rightarrow q_0 = q_N \]

\[ \theta = \frac{2\pi}{N} \{ 0, 1, 2, \ldots, N-1 \} \]

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N dim matrix now has N eigenvalues as expected.
Project: P9

Recover N = 2 case \( w = 0 \)

\[ w = \sqrt{\frac{2k}{m}} \]

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

\[ w^2 = \frac{2k}{m} [1 - \cos q] = 0, \quad \frac{4k}{m} \]

Looks a bit different!

Why?

PBC gives exact

Spring \( k \) between 1, \( N \)

\( N = 2 \) case \( k \) is doubled

Normal modes of 4 masses

\[ w^2 = \frac{2k}{m} [1 - \cos q] = 0, \quad \frac{2k}{m}, \quad \frac{4k}{m}, \quad \frac{2k}{m} \]

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

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Pictorially

Actually usually allow \( q \in [-\pi, \pi] \)

Now do case of 2 different atoms, masses \( M_1, M_2 \)

\[
\begin{align*}
\text{odd} & \quad M_1 X_n = -k(X_n - X_{n+1}) - k(X_n - X_{n-1}) \\
\text{even} & \quad M_2 X_n = -k(X_n - X_{n+1}) - k(X_n - X_{n-1})
\end{align*}
\]

again assume all \( X_n \) (odd and even) have same \( w \)

\[
X_{n(t)} = \begin{cases} a_n e^{iwt} & \text{odd} \\ b_n e^{iwt} & \text{even} \end{cases}
\]

but let amplitudes be different for odd, even

\[
\begin{align*}
a_n &= a_0 e^{i\phi_n} \\
b_n &= b_0 e^{i\phi_n}
\end{align*}
\]

like same \( w \): same \( \phi \)

just different amplitude

DIVOCA
Two eigen result

n odd: \[-M_1 w^2 a_0 = -k(a_0 - b_0 e^{i\theta}) - k(b_0 a_0 e^{-i\theta})\]

n even: \[-M_2 w^2 b_0 = -k(b_0 - a_0 e^{i\theta}) - k(b_0 - a_0 e^{-i\theta})\]

\[
\begin{pmatrix}
2k - M_1 w^2 & -2k \cos \theta \\
-2k \cos \theta & 2k - M_2 w^2
\end{pmatrix}
\begin{pmatrix}
a_0 \\
b_0
\end{pmatrix}
= \begin{pmatrix}0 \\
0\end{pmatrix}
\]

What must happen? \quad \text{new} \quad n = 11 = 0

\[
(2k - M_1 w^2)(2k - M_2 w^2) - 4k^2 \cos^2 \theta = 0
\]

\[
M_1 M_2 w^4 - 2k(M_1 + M_2) w^2 + 4k^2(1 - \cos^2 \theta) = 0
\]

\[
\theta = \frac{11}{2} \quad \text{FIRST} \quad \rightarrow 0
\]

\[
\begin{align*}
1 &= \cos^2 \theta + \sin^2 \theta \\
2 \sin^2 \frac{\theta}{2} &= \cos \theta = \cos^2 \theta - \sin^2 \theta
\end{align*}
\]

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

\[\text{Do NOT COMPLETE} \ldots\]

General comments on strategy:

Normal modes are diagonalize matrix

K-space often does it, or almost does it (after

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2x2 matrix)
Counting?

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

Instead $q$ is now restricted to $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ ($\frac{\pi}{2}$ allowed values), one way to see is that repeated unit is pair of atoms $\circ \quad \rightleftharpoons \quad \circ \quad M_1 \quad \rightleftharpoons \quad M_2$

\[ w^2 \]

\[ 4k/M \]

\[ 2k/M \]

\[ q \]

\[ \frac{\pi}{2} \]

\[ \frac{\pi}{2} \]

\[ \pi \]

\[ \pi \]

\[ 2k/M \]

\[ 2k/M_1 \]

\[ 2k/M_2 \]

\[ \frac{\pi}{2} \]

\[ -\frac{\pi}{2} \]

\[ \frac{\pi}{2} \]

\[ -\frac{\pi}{2} \]

$M_1 = N_1$ case can also be regarded with "folded" zone

(same exact set of $w^2$)

allows better connection $\rightarrow M_1 \neq N_2$ case where $q \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$

$\frac{2k(M_1 M_2)}{M_1 M_2}$

$2k/M_1 \rightarrow \triangle w^1 \rightarrow \triangle w^2$

$2k/M_2 \rightarrow \triangle w^1 \rightarrow \triangle w^2$

DIAGA

key point is gap opens in spectrum.

Some with $m$ $\rightarrow$ moving on lattice of nuclei $\rightarrow$ bond insulators
Do limiting cases first: \( q = 0 \) \( \cos q = 1 \)

\[
(2k - M_1 w^2)(2k - M_2 w^2) - 4k^2 = 0
\]

\[
M_1 M_2 w^4 - 2k(M_1 + M_2) w^2 = 0
\]

\[
w^2 (w^2 M_1 M_2 - 2k(M_1 + M_2)) = 0
\]

1) \( w^2 = 0 \)

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

\( q = \frac{\pi}{2} \) \( \cos q = 0 \)

\[
M_1 M_2 w^4 - 2k(M_1 + M_2) w^2 + \frac{4k^2}{4} = 0
\]

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

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

\[
w = \frac{K}{M_1 M_2} \left[ M_1 + M_2 \pm (M_1 - M_2) \right] \rightarrow \frac{2k}{M_2}
\]

\[
w = \frac{K}{M_1 M_2} \left[ M_1 + M_2 \pm (M_1 - M_2) \right] \rightarrow \frac{2k}{M_1}
\]
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 these dispersion relations intersect/overlap

Reason: Energy and momentum match up

\[
\gamma \rightarrow k' \omega' \leftarrow \gamma
\]

for acoustic phonons

if photon & beams

\( \omega = c(k-k') \)

associated energy \( \omega - \omega' n c (k-k') \)

is likely to be way more than

acoustic phonon can accommodate.
What changes in 3D? Very little.

Basically 2 modes

optic / acoustic $\rightarrow$ 6 modes

(3 optic, 3 acoustic)

because atoms can vibrate in 3 directions

$x \rightarrow x, y, z$

Often label modes longitudinal vs transverse

according to whether displacement is $\parallel$ or $\perp$ to

propagating direction

\[
\begin{cases}
\text{vibrating string} & \text{transverse} \\
\text{sound in pipe (compression wave)} & \text{longitudinal}
\end{cases}
\]

bulk vs shear modulus

$\rightarrow$ building properties

steel girder vs concrete

\[E(r) = E_0 e^{ik \cdot r} \quad \nabla \cdot \mathbf{E} = 0\]

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

Triatomic molecule:

\[ m \quad m \quad m \]

\[ k \quad k \]

\[ m x_1 = -k(x_1 - x_2) \]

\[ m x_2 = -k(x_2 - x_1) - (x_2 - x_3) \]

\[ x_0(t) = q_n e^{i\omega t} \]

\[ m x_3 = -k(x_3 - x_2) \]

\[
\begin{bmatrix}
  1 & -1 & 0 \\
  -1 & 2 & -1 \\
  0 & -1 & 1 \\
\end{bmatrix}
\begin{bmatrix}
  q_1 \\
  q_2 \\
  q_3 \\
\end{bmatrix}
= \omega^2
\begin{bmatrix}
  q_1 \\
  q_2 \\
  q_3 \\
\end{bmatrix}
\]

\[ \vec{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \omega^2 = 0 \]

\[ \vec{v}_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \omega^2 = \frac{k}{m} \quad \text{Similar to HW problem} \quad \text{central mass doesn't move} \]

\[ \vec{v}_3 = \begin{pmatrix} 1 \\ -2 \end{pmatrix} \quad \omega^2 = \frac{3k}{m} \]
The problem points out some interesting modes of \( M_1, M_2 \) system.

\[ M_1 \leftarrow k \rightarrow M_2 \leftarrow k \rightarrow M_1 \]

\[ M_2 \text{ at rest: obviously } w^2 = \frac{2k}{m_1} \]

Likewise \( M_1 \) at rest.

This case comes out of our general solution.

In fact they are part of \( M_1 = M_2 \) case.

\[
\begin{bmatrix}
2 & -1 & 0 & 0 & 0 & -1 \\
-1 & 2 & -1 & 0 & 0 & 0 \\
K/m & 0 & -1 & 2 & -1 & 0 \\
\end{bmatrix}
\]

Before we discussed \( \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \)

But note \( \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \)

\[ \text{eigen} \rightarrow \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \]

\[ q = 0 \]

\[ q = \pi \]

\% = \frac{\pi}{2} \text{ and } -\frac{\pi}{2} \text{ are degenerate}\]
More connections:

- Vibrating strings have nodes.

Analog: is this mode has same \( w^2 \) when \( M_2 \neq M_1 \). Since \( M_2 \) never moves, \( w^2 \) unchanged.

- In QM class, \( \psi \) for square well, perturbation of \( V \delta(x-a) \).

If \( a \) is at node of \( \phi_n \), \( \phi_n \) is eigenstate of \( H' \), then \( E_n = 0 \); no energy shift.
Time independent Schrödinger Eqn

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

Laplace/Poisson Eqn

\[-\nabla^2 \phi(x) = \rho(x) / \varepsilon_0\]

\[E = -\nabla \phi\]

\[\nabla \cdot E = \rho / \varepsilon_0\]

Diffusion Eqn

\[\frac{\partial p(x,t)}{\partial t} = \kappa \nabla^2 p(x,t)\]

So $\nabla^2$ ubiquitous QM, EM, CM

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

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

\[
\begin{bmatrix}
-1 & 2 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
f((n+1)\Delta x) \\
f(n\Delta x) \\
f((n-1)\Delta x) \\
\end{bmatrix}
\]