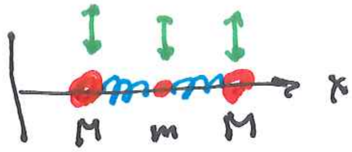
More complex normal mode problems — add wiggle to stretch



add y motion to CO_2 problem
need a restoring force related to

angle with an equilibrium point at $\theta = 180$ & larger PE as move away from straight.

Cross product of CO bonds provides something 0 when straight and a difference (which we can square) when bent.

$$\overrightarrow{r_1 - r_2} \times \overrightarrow{r_3 - r_2} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x_1 - x_2 - l & y_1 - y_2 & 0 \\ x_3 - x_2 + l & y_3 - y_2 & 0 \end{vmatrix} = \begin{matrix} (x_1 - x_2 - l)(y_3 - y_2) \\ - (x_3 - x_2 + l)(y_1 - y_2) \end{matrix}$$

$$= -l\left[y_3 + y_1 - 2y_2\right] + \text{terms } \overbrace{x \cdot y}^{\text{neglect}}$$

$$\Rightarrow PE \propto \frac{1}{2} k_y \left(y_3 + y_1 - 2y_2\right)^2$$

Overall: $T = \frac{1}{2}\left[M\dot{x}_1^2 + m\dot{x}_2^2 + M\dot{x}_3^2 + M\dot{y}_1^2 + m\dot{y}_2^2 + M\dot{y}_3^2\right]$

$$U = \frac{1}{2} k_x \left[(x_2 - x_1)^2 + (x_3 - x_2)^2\right] + \frac{1}{2} k_y \left[y_3 + y_1 - 2y_2\right]^2$$

$$U = \frac{1}{2} k_x \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \underbrace{\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}}_{\frac{\partial^2 u}{\partial x_i \partial x_j}} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \frac{1}{2} k_y \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \underbrace{\begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix}}_{\frac{\partial^2 u}{\partial y_i \partial y_j}} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

Note: I've written x & y as separate vectors/matrices but the plan is to put together a big 6x6 matrix

$$U = \frac{1}{2} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} \left(\begin{array}{c|c} k_x \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} & 0 \\ \hline 0 & k_y \begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix} \end{array} \right) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

But we need to do something else first.

```
U=kx/2( (q[2]-q[1])^2+(q[3]-q[2])^2)+ky/2(q[6]+q[4]-2 q[5])^2
U2=U /. {q[2]->Sqrt[M/m] q[2],q[5]->Sqrt[M/m] q[5]}
k=Table[Table[ D[U2,q[i],q[j]],{j,1,6}],{i,1,6}]
eigen=Eigensystem[k]
```

Note to get actual ω^2 divide by M

```
                           kx (m + 2 M)  2 (ky m + 2 ky M)
Out[4]= {{0, 0, 0, kx, ------------, -----------------}, cut
                                m                 m
```

usual

new bending mode

undo scale change

```
tx=IdentityMatrix[6]
tx[[2,2]]=Sqrt[M/m]
tx[[5,5]]=Sqrt[M/m]

Last[eigen].tx
```

rotation

rotation + translation

```
                                                     M        M
Out[8]= {{0, 0, 0, -1, 0, 1}, {0, 0, 0, 2 Sqrt[-], Sqrt[-], 0},
                                                     m        m
```

translation

```
                                                          -2 M
>     {1, 1, 1, 0, 0, 0}, {-1, 0, 1, 0, 0, 0}, {1, ----, 1, 0, 0, 0},
                                                           m
```

usual

see

```
                  -2 M
>     {0, 0, 0, 1, ----, 1}}
                   m
```

new bending

```
CO2
2438.1 cm^-1
1373.01
641.49
* ? 1+32/12
    3.666666666666667
* ? (2438/1373)^2
    3.153017114478638


Ge O2
1061.6
870.1
195.5

 ? 1+32/72.6
    1.440771349862259
* ? (1061.6/870.1)^2
    1.488618741515112
```

The only pleasant way to solve 6x6 matrix problems is with Mathematica (but see below). Mathematica is willing & able to solve Eigensystem problems - but this is not exactly an eigensystem because the mass matrix $\begin{bmatrix} M & & & & & \\ & m & & & & \\ & & M & & & \\ & & & M & & \\ & & & & m & \\ & & & & & M \end{bmatrix}$ is not a scalar multiple of the unit matrix.

Solution - make a change in variables to make the mass matrix $= M\overleftrightarrow{1}$. Let $x_2 = \sqrt{\frac{M}{m}}\, q_2$ so $\frac{1}{2} m \dot{x}_2^2 = \frac{1}{2} M \dot{q}_2^2$ & $y_2 = \sqrt{\frac{M}{m}}\, q_5 \Rightarrow (x_i \;\&\; y_i) \to q_i$

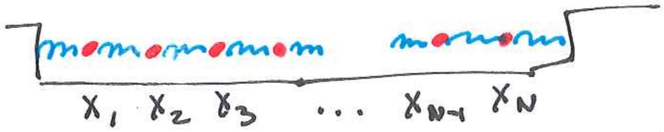
Make above substitutions into PE then take $\frac{\partial^2 U}{\partial q_i \partial q_j}$ to find the K matrix ... $L = \frac{1}{2} M \dot{\vec{q}}\, \overleftrightarrow{1}\, \dot{\vec{q}} - \frac{1}{2} \vec{q}\, [K]\, \vec{q}$

Lagrange $\Rightarrow$ $M \ddot{\vec{q}} = -[K]\vec{q}$ try $\vec{q} = \vec{a}\, e^{i\omega t}$ ← constant

$$\underbrace{M\omega^2}_{\text{exactly an eigenvalue of } [K]} \vec{a} = [K]\vec{a}$$

Note: to get the physical locations x & y : $x_2 = \sqrt{\frac{M}{m}}\, q_2$ etc

Now lets solve an arbitrarily large matrix problem by hand.



N masses m connected with identical springs

$$T = \frac{1}{2}\sum_{j=1}^{N} m \, \dot{x}_j^2 \qquad U = \frac{1}{2} k \left[\sum_{j=0}^{N} (x_{j+1} - x_j)^2 \right]$$

where $x_0 = 0$

$x_{N+1} = 0$ [from offset]

mass matrix $= m \, \mathbb{1}$

Note every x_j (except 0 & N+1) appears twice

$(x_{j+1} - x_j)^2 + (x_j - x_{j-1})^2$

mixed partial $\frac{\partial}{\partial x_j \partial_{j+1}}$ $\longleftarrow$ $\frac{\partial}{\partial x_j} \Rightarrow 2(x_{j+1} - x_j)(-1) + 2(x_j - x_{j-1})$

with either j+1 or j-1

$\Rightarrow$ -2

$$\frac{\partial^2}{\partial x_j} \Rightarrow 2 + 2 = 4$$

just off diagonal = -1

Note overall factor of $\frac{1}{2}k \Rightarrow$

$$[K] = k \begin{bmatrix} -1 & 2 & -1 & & 0 \\ & -1 & 2 & -1 & \\ 0 & & -1 & 2 & -1 \end{bmatrix}$$

main diagonal has 2

Lagrange $\Rightarrow \quad m \, \mathbb{1} \begin{pmatrix} \ddot{x} \end{pmatrix} = -k \begin{bmatrix} \; \end{bmatrix} \begin{pmatrix} x \end{pmatrix}$

Try $\begin{pmatrix} x \end{pmatrix} = \vec{a} \, e^{i\omega t}$

$\uparrow$ constant

$\Rightarrow \quad m\omega^2 \, \mathbb{1} \, \vec{a} = k \begin{bmatrix} \; \end{bmatrix} \vec{a}$

since $\frac{k}{m}$ is usual $\omega_0^2 \Rightarrow \frac{\omega^2}{\omega_0^2} = \lambda =$ eigenvalue

$$\lambda \vec{a} = \begin{bmatrix} \; \end{bmatrix} \vec{a}$$

$$\lambda a_j = -a_{j-1} + 2a_j - a_{j+1}$$ $\leftarrow$ linear

new factor

Try $a_j = \text{Re}\left[A e^{ij\gamma} \right]$

$\Rightarrow \lambda = -e^{-i\gamma} + 2 - e^{+i\gamma}$ $\quad \leftarrow A e^{ij\gamma}$ is common to all

$$= 2(\underbrace{1 - \cos\gamma}_{= 2\sin^2\frac{\gamma}{2}}) = 4\sin^2\left(\frac{\gamma}{2}\right)$$

BC are going to tell us what γ are possible!

$$x_0 = \mathrm{Re}\left[A e^{i0}\right] = 0 \Rightarrow A = \text{pure imaginary eg } i$$

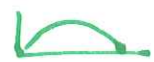
$$x_{N+1} = \mathrm{Re}\left[A e^{i(N+1)\gamma}\right] = 0 \Rightarrow e^{i(N+1)\gamma} \text{ pure real}$$

only possible if $(N+1)\gamma = s\pi$

integer

$$\therefore \gamma = \frac{s\pi}{N+1} \qquad s = 1, 2, \cdots, N$$

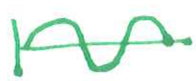
if $s=1$ $\quad j\gamma = \frac{j}{N+1}\pi$ will go $\underbrace{0 \rightarrow \pi}_{\frac{1}{2}\text{ cycle}}$ as j goes $1 \rightarrow N$

$\frac{1}{2}$ cycle : 

if $s=2$ $\quad j\gamma = \frac{j}{N+1} 2\pi$ will go $\underbrace{0 \rightarrow 2\pi}_{\text{full cycle}}$ as j goes $1 \rightarrow N$

full cycle 

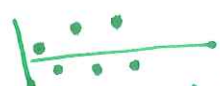
if $s=3$ $\quad j\gamma = \frac{j}{N+1} 3\pi$ will go $\underbrace{0 \rightarrow 3\pi}$ as j goes $1 \rightarrow N$



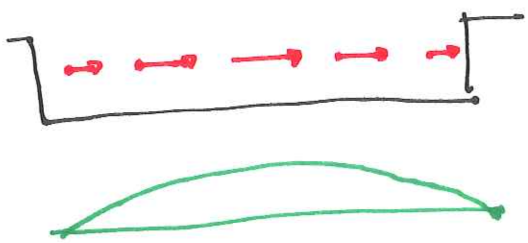
conclude s is # half cycles as j goes $1 \rightarrow N$

⋮

if $s = N$ $\quad \gamma = \frac{N}{N+1}\pi \approx \pi$ so $e^{ij\gamma}$ will alternate.



etc

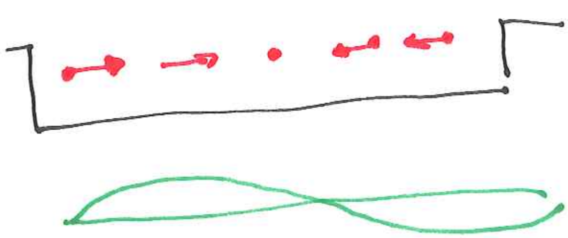
$s=1$: 

$$\lambda = \frac{\omega^2}{\omega_0^2} = 4\sin^2\left(\frac{\gamma}{2}\right)$$

$$\approx \gamma^2 = \left[\frac{s\pi}{N+1}\right]^2$$

$$\omega \approx \omega_0 \left[\frac{s\pi}{N+1}\right]$$

much lower freq than ω_0 cuz adjacent particles move together

$s=2$ 

I hope this reminds you of resonance in a closed-closed organ pipe because that's exactly what it is.