$$L = \frac{1}{2} m_{ij}(\tilde{q})\, \dot{\tilde{q}}^i \dot{\tilde{q}}^j - U(\tilde{q})$$

so expand around equilibrium:

$$\tilde{q}^i = \underset{\substack{\text{Equilibrium} \\ \text{constant}}}{q_0^i} + \underset{\substack{\text{Displacement} \\ \text{from equilibrium.}}}{q^i}$$

$$U(\tilde{q}) = U(q_0) + \cancel{\left(\frac{\partial U}{\partial \tilde{q}^i}\right)} q^i + \frac{1}{2} \underbrace{\left(\frac{\partial^2 U}{\partial \tilde{q}^i \partial \tilde{q}^j}\right)}_{K_{ij}} q^i q^j$$

if at minimum

$$\frac{\partial U}{\partial \tilde{q}^i} = 0$$

$$L = \frac{1}{2} m_{ij}\, \dot{q}^i \dot{q}^j - \frac{1}{2} K_{ij}\, q^i q^j$$

then EOM:

$$m_{ij} \ddot{q}^j = -K_{ij} q^j$$

Try ansatz: $q^j(t) = \underline{E}^j e^{-i\omega t}$

$$\dot{q}^j = -i\omega \underline{E}^j e^{-i\omega t}$$
$$\ddot{q}^j = -\omega^2 \underline{E}^j e^{-i\omega t}$$

$$\hookrightarrow -\omega^2 m_{ij} \underline{E}^j = -K_{ij} \underline{E}^j$$

let $\mathbb{K} = (k_{ij})$ $\quad M = m_{ij}$ $\quad E^j = \begin{pmatrix} E^1 \\ E^2 \\ \vdots \end{pmatrix}$ → Eigenvectors.

↳ $(K - \omega^2 M) E^j = 0.$

$\det(K - \omega^2 M) = 0$ leads to nontrivial solution.

Finds a polynomial of degree n, for ω^2, $P(\omega^2) = 0$

Eigenvalue of the system.

Once we know ω_a^2, find each $E_a{}^j$ after plug in ω_a^2.

Form a complete solution:

$$q^j(t) = \sum_{a=1}^{N} C_+^a E_a{}^j e^{-i\omega_a t} + C_-^a E_a{}^j e^{+i\omega_a t}$$

Adjust C_+ and C_- to reproduce $q^j(t=0)$ and $\dot{q}^j(t=0)$

<u>Generalized eigenvalue problem:</u>

$$K \vec{E} = \omega^2 M \vec{E} \quad \text{vs} \quad K\vec{E} = \lambda \vec{E}$$

generalized case.

$K^\dagger = (\bar{K})^T$ ← take conjugate then transpose.

let K to be Hermitian, $K = K^\dagger$

M to be definite positive symmetric.

properties:

$$\boxed{\begin{array}{l} \text{① Eigenvalues are real} \\ \text{② The eigenvectors are orthogonal with } M \text{ as weight.} \overset{\text{or}}{\Rightarrow} \vec{E}_a M \vec{E}_b = E_a^{i*} M_{ij} E_b^j = \delta_{ab} \end{array}}$$

Inner product: $(\vec{X}, \vec{Y}) = (X^{i*}) Y^i$ ← Cartesian Inner Product.

Weighted Inner product: $(\vec{X}, W\vec{Y}) = X^{*i} W_{ij} Y^j$

For M is positive and definite:

$$(\vec{X}, M\vec{X}) \geq 0$$

then $$(\vec{E}_a, M\vec{E}_b) = 0 \quad \text{for } a \neq b.$$

Change of basis:

$$\boxed{q^j(t) = Q^a(t)\, E_a^j}$$

then
$$U = \frac{1}{2} k_{ij}\, q^i q^j$$
$$\stackrel{!}{=} \frac{1}{2} k_{ij}\, Q^a(t) E_a^i\, Q^b(t) E_b^j$$
$$\stackrel{!}{=} \frac{1}{2} Q^a(t) Q^b(t)\, E_a^i \underbrace{k_{ij} E_b^j}_{= \omega_b^2 m_{ij} E_b^j}$$
$$\stackrel{!}{=} \frac{1}{2} Q^a(t) Q^b(t) \omega_b^2\, \underbrace{E_a^i m_{ij} E_b^j}_{}$$

δ_{ab} ↖ $*$

$$= \frac{1}{2}\sum_a (Q^a)^2 \omega_a^2$$

$$T = \frac{1}{2} m_{ij} \dot{q}^i \dot{q}^j = \frac{1}{2}\sum_{ab} \dot{Q}^a \dot{Q}^b \underbrace{E_a^{\ i} m_{ij} E^j_{\ b}}_{\delta_{ab}}$$

$$= \frac{1}{2}\sum_a (\dot{Q}^a)^2$$

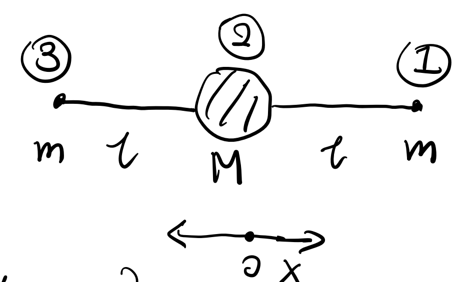
then

$$L = \sum_a \frac{1}{2}(\dot{Q}^a)^2 - \frac{1}{2}\omega_a^2 (Q^a)^2$$

$$\ddot{Q}^a = -\omega_a^2 Q^a$$ ← decoupled, diagonalized SHO.

For $Q^a = C_+^a e^{i\omega_a t} + C_-^a e^{-i\omega_a t}$

Ex:



$$\left.\begin{aligned} x_1 &= l + u_1 \\ x_2 &= u_2 \\ x_3 &= -l + u_3 \end{aligned}\right\}$$ u is a small displacement.

$$T = \frac{1}{2} m \dot{u}_1^2 + \frac{1}{2} M \dot{u}_2^2 + \frac{1}{2} m \dot{u}_3^2$$

$$U = \frac{1}{2}k(u_1 - u_2)^2 + \frac{1}{2}k(u_2 - u_3)^2$$

$$= \frac{1}{2}k(u_1^2 - 2u_1 u_2 + u_2^2) + \frac{1}{2}k(u_2^2 - 2u_2 u_3 + u_3^2)$$

<u>EOM:</u>

$$\underbrace{\begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix}}_{M} \begin{pmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \ddot{u}_3 \end{pmatrix} = - \underbrace{\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}}_{K} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

$$M\ddot{u} = -K u$$

let $\vec{u} = \vec{E} e^{-i\omega t}$

$$-M\omega^2 \vec{E} = -K \vec{E}$$

$$(-M\omega^2 + K)\vec{E} = 0$$

$$\det\left[\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} - \begin{pmatrix} m\omega^2 & 0 & 0 \\ 0 & M\omega^2 & 0 \\ 0 & 0 & m\omega^2 \end{pmatrix}\right] = 0$$

$$(k-m\omega^2)\left[(2k-M\omega^2)(k-m\omega^2) - k^2\right]$$
$$- k^2\left[k - m\omega^2\right]$$

$$= (k-m\omega^2)\left[\underset{k^2}{2k^2} - 2km\omega^2 - kM\omega^2 + mM\omega^4 - \cancel{k^2}\right] - k^3 + k^2 m\omega^2$$

$$\stackrel{!}{=} k^3 - 2k^2 m\omega^2 - k^2 M\omega^2 + mM\omega^4 k - \cancel{k^3}$$
$$- k^2 m\omega^2 + 2km^2\omega^4 + kmM\omega^4 - m^2 M\omega^6 + k^2 m\omega^2$$

$$\stackrel{!}{=} -m^2 M\omega^6 + (2km^2 + 2kmM)\omega^4 - \omega^2(3k^2 m + k^2 M)$$

$$\omega^2\left(-m^2M\omega^4 + 2km(m+M)\omega^2 - (2m+M)k^2\right)$$

$$\omega^2 = \frac{-\cancel{2}k\cancel{m}(m+M) \pm \sqrt{\cancel{4}k^2\cancel{m^2}(m+M)^2 - \cancel{4}\,\cancel{m^2}M(2m+M)k^2}}{-\cancel{2}\,m^{\cancel{2}}M}$$

$$\stackrel{!}{=} k\left[\frac{-(m+M) \pm \sqrt{m^2 + \cancel{2mM} + \cancel{M^2} - \cancel{2mM} - M^2}}{-mM}\right]$$

$$\stackrel{!}{=} k\left[\frac{-(m+M) \pm m}{-mM}\right]$$

$$\omega_+^2 = k/m \qquad \omega_-^2 = k\left[\frac{2m+M}{mM}\right]$$

$$\omega_-^2 \stackrel{!}{=} \frac{k}{m}\left(1 + \frac{2m}{M}\right)$$

$$\omega_0^2 = 0$$

Find eigenvectors

$\underline{\omega_0^2 = 0}$

$$\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}\begin{pmatrix} E_1^0 \\ E_2^0 \\ E_3^0 \end{pmatrix} \Rightarrow \begin{array}{l} E_1^0 = E_2^0 \\ E_2^0 = E_3^0 \end{array}$$

$$E^0 = (1, 1, 1)$$

$$\omega_+^2 = k/m$$

$$\left[\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} - \begin{pmatrix} m\frac{k}{m} & 0 & 0 \\ 0 & M\frac{k}{m} & 0 \\ 0 & 0 & m\frac{k}{m} \end{pmatrix}\right]\begin{pmatrix} E_1^+ \\ E_2^+ \\ E_3^+ \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -k & 0 \\ -k & 2k-\frac{kM}{m} & -k \\ 0 & -k & 0 \end{pmatrix}\begin{pmatrix} E_1^+ \\ E_2^+ \\ E_3^+ \end{pmatrix}$$

$$\hookrightarrow \; -kE_2^+ = 0 \quad \Rightarrow \quad E_2^+ = 0$$

$$-kE_1^+ + \underbrace{\cancel{\left(2k-\frac{kM}{m}\right)E_2^+}}_{0} - kE_3^+ = 0$$

$$-E_1^+ = E_3^+$$

let $E_1^+ = 1$, then $E_3^+ = -1$

$$E^+ = (1, 0, -1)$$

$$\omega_-^2 = \frac{k}{m}\left(1 + \frac{2m}{M}\right)$$

$$\left[\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \end{pmatrix} - \begin{pmatrix} m\frac{k}{m}\left(1+\frac{2m}{M}\right) & 0 & 0 \\ 0 & M\frac{k}{m}\left(1+\frac{2m}{M}\right) & 0 \end{pmatrix}\right]\begin{pmatrix} E_1^- \\ E_2^- \end{pmatrix}$$

$$\begin{bmatrix} 0 & -k & k \end{bmatrix} \quad \begin{bmatrix} 0 & 0 & m\frac{k}{m}\left(1+\frac{2m}{M}\right) \end{bmatrix} \quad \begin{bmatrix} \bar{E}_3 \end{bmatrix}$$

$$\begin{pmatrix} -k\frac{2m}{M} & -k & 0 \\ -k & 2k-\frac{kM}{m}\left(1+\frac{2m}{M}\right) & 0 \\ 0 & -k & -k\left(\frac{2m}{M}\right) \end{pmatrix} \begin{pmatrix} \bar{E}_1 \\ \bar{E}_2 \\ \bar{E}_3 \end{pmatrix}$$

$$\hookrightarrow \quad -\cancel{k}\frac{2m}{M}\bar{E}_1 - \cancel{k}\bar{E}_2 = 0.$$

$$\frac{2m}{M}\bar{E}_1 = -\bar{E}_2$$

$$E_1 = 1 \Rightarrow \bar{E}_2 = -\frac{2m}{M}$$

$$-k\bar{E}_2 - k\left(\frac{2m}{M}\right)\bar{E}_3 = 0.$$

$$-\bar{E}_2 = \frac{2m}{M}\bar{E}_3$$

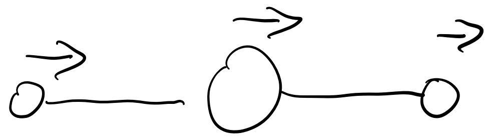
let $\bar{E}_2 = \frac{-2m}{M} \Rightarrow \bar{E}_3 = 1.$

$$\bar{E} = \left(1, \frac{-2m}{M}, 1\right)$$

$$\omega_a^2 = 0, \frac{k}{m}, \frac{k}{m}\left(1+\frac{2m}{M}\right)$$

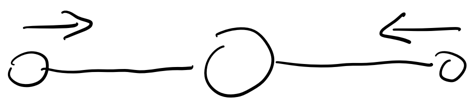
$$E = (1, 1, 1) \quad (1, 0, -1) \quad \left(1, \frac{-2m}{M}, 1\right)$$

0^{th} Mode:

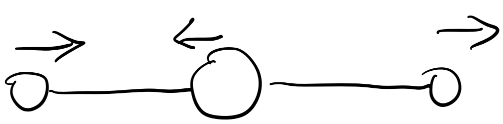


displace by same amount

<u>+ mode:</u>



<u>− mode:</u>



Check orthogonality:

$$\vec{E}_0 M \vec{E}_2 = (1 \ 1 \ 1)\begin{pmatrix} m & & \\ & M & \\ & & m \end{pmatrix}\begin{pmatrix} 1 \\ \frac{-2m}{M} \\ 1 \end{pmatrix}$$

$$\stackrel{!}{=} m - 2m + m = 0$$

And vector can be combination of 3 modes:

$$\vec{u} = \vec{E}_1 Q^1(t) + \vec{E}_2 Q^2(t) + \vec{E}_3 Q^3(t)$$

For EOM: $\ddot{Q} = -\omega_a^2 Q^a$

So $Q(t) = A\cos\omega_a t + B\sin\omega_a t$ for $\omega_a \neq 0$

$= A + Bt$ for $\omega_a = 0$

$$\omega_a^2 = 0, \quad \frac{k}{m}, \quad \frac{k}{m}\left(1+\frac{2m}{M}\right)$$

$$E = (1,1,1) \quad (1,0,-1) \quad \left(1, \frac{-2m}{M}, 1\right)$$

$$\tilde{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = (A+Bt)\begin{pmatrix} E_1^0 \\ E_2^0 \\ E_3^0 \end{pmatrix} + A_1\cos(\omega_1 t+\phi_1)\begin{pmatrix} E_1^1 \\ E_2^1 \\ E_3^1 \end{pmatrix} + A_2\cos(\omega_2 t+\phi_2)\begin{pmatrix} E_1^2 \\ E_2^2 \\ E_3^2 \end{pmatrix}$$

Zero Mode:

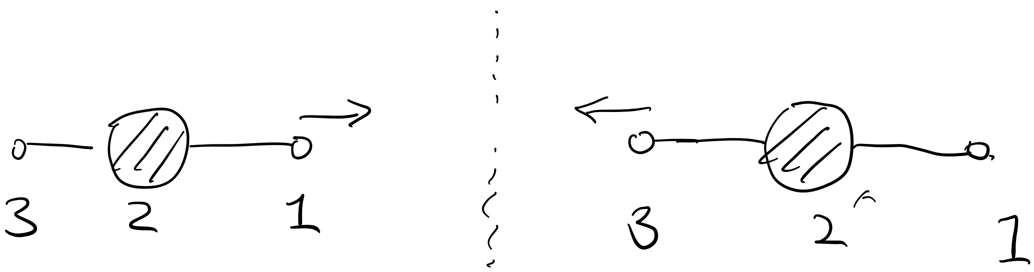
→ shift in center of mass. $(1, 1, 1)$

→ Orthognality to $E_0 = (1,1,1)$ means, that center of mass shift $= 0$.

$$(1, 1, 1)\begin{pmatrix} m & & \\ & M & \\ & & m \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

$$m x_1 + M x_2 + m x_3 = 0$$

Symmetry Thinking :



$(1,0,0)$ $(0,0,-1)$

given $\vec{x} = (x_1, x_2, x_3)$ here x_i are the ith particle.

$$\vec{x} \rightarrow \tilde{\underline{x}} = (\underline{x}_1, \underline{x}_2, \underline{x}_3) = (-x_3, -x_2, -x_1)$$

Reflection of $\tilde{x}$

Even mode if: $\tilde{\underline{x}} = \vec{x} \Rightarrow (\underline{x}_1, \underline{x}_2, \underline{x}_3) = (x_1, x_2, x_3)$

Odd mode if: $\tilde{\underline{x}} = -\tilde{x} \Rightarrow (\underline{x}_1, \underline{x}_2, \underline{x}_3) = -(x_1, x_2, x_3)$

So

For odd: $(\underline{x}_1, \underline{x}_2, \underline{x}_3) \overset{\text{general}}{=} -x_3, -x_2, -x_1$

$$\overset{!}{=} -x_1, -x_2, -x_3$$

$-x_3 = -x_1$?

$$-x_2 = -x_2$$
$$-x_1 = -x_3 \quad \Big\} \quad \text{so} \quad x_1 = x_3$$

For even: $(x_1, x_2, x_3) = -x_3, -x_2, -x_1$
$$= x_1, x_2, x_3$$

$$-x_3 = x_1$$
$$-x_2 = x_2$$
$$-x_1 = x_3$$

We had one even mode:

$$(x_1, x_2, x_3)_{even} = q(t)_{even}\,(-1, 0, 1)$$

Then odd mode:

since $x_1 = x_3$

$$(x_1, x_2, x_3)_{odd} = \left(q_3, q_2, q_3\right)$$

The zeroth mode: (shift in center of mass).

$$\vec{x}_0 = q_{cm}\,(1, 1, 1)$$

Choose our coordinate to be orthogonal to $\vec{x}_0$

$(1 \quad 1 \quad 1)/m \qquad \Big| \Big(q_3 \Big|$

$$\begin{pmatrix} & & \\ & M & \\ & & m \end{pmatrix}\begin{pmatrix} \\ q_2 \\ q_3 \end{pmatrix} = 0$$

$$2mq_3 + Mq_2 = 0 \quad \Rightarrow \quad q_2 = \frac{-2m}{M} q_3$$

then for $q_3 = 1$

$$\hookrightarrow q_2 = \frac{-2m}{M}$$

$$(q_3, q_2, q_3) = q_{cm}(1,1,1) + q_0\left(1, \frac{-2m}{M}, 1\right)$$

Change of basis:

$$\vec{u} = u_1(1,0,0) + u_2(0,1,0) + u_3(0,0,1)$$
$$= q^e(-1,0,1) + q^0\left(1, \frac{-2m}{M}, 1\right) + q_{cm}(1,1,1)$$

then:

$$u_1 = -q^e + q^0 + q_{cm}$$

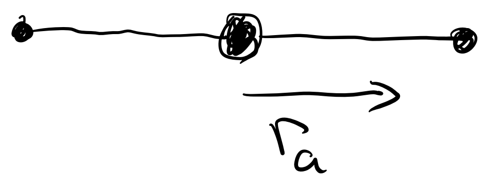
$$u_2 = \frac{-2m}{M} q^0 + q_{cm}$$

$$u_3 = q^e + q^0 + q_{cm}$$

$$\mathcal{L} = \frac{1}{2}m\dot{u}_1^2 + \frac{1}{2}M\dot{u}_2^2 + \frac{1}{2}m\dot{u}_3^2 - \frac{1}{2}k(u_1 - u_2)^2 - \frac{1}{2}k(u_2 - u_3)^2$$

$$= \underbrace{\frac{1}{2} M \dot{q}_{cm}^{2}}_{\text{CoM motion}} + \underbrace{m \dot{q}_e^{2} - k q_e^{2}}_{\text{Even oscillation}} + \underbrace{\frac{m(2m+M)}{M} \dot{q}_o^{2} - \frac{k(2m+M)^2}{M^2} q_o^{2}}_{\text{odd oscillations}}$$

Ex: 3D Molecules.



$$\vec{r}_a = \vec{r}_{eq} + \delta \vec{r}_a$$

then displacements:

$$Y = (\delta \vec{r}_1, \delta \vec{r}_2, \delta \vec{r}_3)$$

There are 3-translational zeroth mode.

$$E_0^X = (1, 1, 1)\hat{X}$$
$$E_0^Y = (1, 1, 1)\hat{Y}$$
$$E_0^Z = (1, 1, 1)\hat{Z}$$

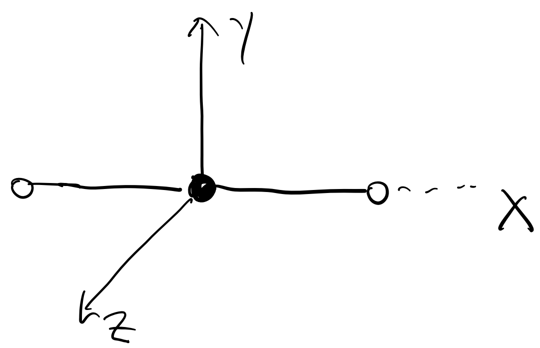
Require X orthogonal to E_0^X:

Y orthogonal to E_0^Y
Z orthogonal to E_0^Z

$$\hookrightarrow m\delta\vec{r}_1 + M\delta\vec{r}_2 + m\delta\vec{r}_3 = 0$$

$$\hookrightarrow mX_1 + MX_2 + mX_3 = 0$$
$$mY_1 + MY_2 + mY_3 = 0$$
$$mZ_1 + MZ_2 + mZ_3 = 0$$

Rotation zero mode:



$$\vec{E}_0 = (\delta\vec{\theta} \times \vec{r}_{eq1},\ \delta\vec{\theta} \times \vec{r}_{eq2},\ \delta\vec{\theta} \times \vec{r}_{eq3})$$

Requires $(\vec{E}_0, M\vec{Y}) = 0$

For $\vec{Y} = (\delta\vec{r}_1, \delta\vec{r}_2, \delta\vec{r}_3)$

$$(\vec{E}_0, M\vec{Y}) = m\,\delta\vec{r}_1 \cdot \delta\vec{\theta} \times \vec{r}_{eq1} + M\,\delta\vec{r}_2 \cdot \delta\vec{\theta} \times \vec{r}_{eq2} + m\,\delta\vec{r}_3 \cdot \delta\vec{\theta} \times \vec{r}_{eq,3} = 0.$$

$$\hookrightarrow \delta\vec{\theta}\cdot\underbrace{\left(m\,\vec{r}_{eq,1}\times\delta\vec{r}_1 + M\,\vec{r}_{eq,2}\times\delta\vec{r}_2 + m\,\vec{r}_{eq,3}\times\delta\vec{r}_3\right)}_{=0.} = 0$$

If take time derivative

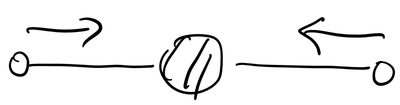
$$m\,\vec{r}_{eq,1}\times\delta\dot{\vec{r}}_1 + M\,\vec{r}_{eq,2}\times\delta\dot{\vec{r}}_2 + m\,\vec{r}_{eq,3}\times\delta\dot{\vec{r}}_3 = 0$$

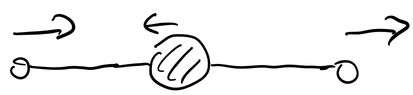
Net angular momentum is zero.

$$\left.\begin{aligned} E_0^z &= l(\hat{y}, 0, -\hat{y}) && \text{rotate about } z \\ E_0^y &= l(-\hat{z}, 0, \hat{z}) && \text{rotate about } y \end{aligned}\right\} \text{2 rotational modes.}$$

$$E_0^x = 0$$

2 vibrational modes in x :

①


②


Vibrational mode in $\hat{y}$:

so $\vec{u} = (y_1, y_2, y_3)\hat{y}$

Use previous normal modes in $\hat{y}$ as constraint:

$$mY_1 + MY_2 + mY_3 = 0 \quad \Leftarrow \text{Translational in } \hat{y}$$

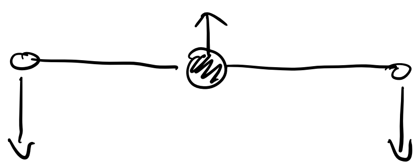
$$(E^z_0, MY) = m\ell Y_1 + 0 - m\ell Y_3 = 0$$

$\hookrightarrow$ so $Y_1 = Y_3 = 1$

$$mY_1 + MY_2 + mY_1 = 0.$$

$$\frac{-2m}{M} Y_1 = Y_2$$

$$E^y_{bend} = Y_{bend}\left(1, \frac{-2m}{M}, 1\right)\hat{y}$$



By symmetry in y and z: vibrational in $\hat{z}$

$$E^z_{bend} = Z_{bend}\left(1, \frac{-2m}{M}, 1\right)\hat{z}$$