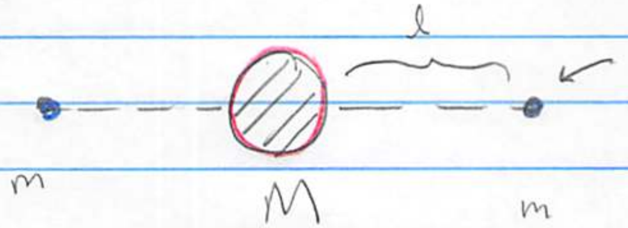
# Tong 2.5.2 - A Linear molecule in 1D

- Consider a linear molecule




← $x_1 = \ell + u_1$ ← linear displacement

- We have three displacements $x_1, x_2, x_3$ and three normal modes. For simplicity assume that the potential is

$$V = V_0(x_1 - x_2) + V_0(x_2 - x_3)$$

So that near the minimum we expand

$$x_1 = \ell + u_1, \quad x_2 = u_2, \quad x_3 = -\ell + u_3$$

- So

$$V \simeq \frac{1}{2} k \left[ (u_1 - u_2)^2 + (u_2 - u_3)^2 \right]$$

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

Then the EOM reads

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

So we look for E-vectors $u^i = E^i e^{-i\omega t}$

$$\underbrace{\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ & -k & k \end{pmatrix}}_{\equiv \mathbb{K}} \begin{pmatrix} E^1 \\ E^2 \\ E^3 \end{pmatrix} = \omega^2 \underbrace{\begin{pmatrix} m & & \\ & M & \\ & & m \end{pmatrix}}_{\equiv \mathbb{M}} \begin{pmatrix} E^1 \\ E^2 \\ E^3 \end{pmatrix}$$

- To find the evectors we either use Eigensystem[{K, M}] in mathematical or find

$$\det(\mathbb{K} - \lambda \mathbb{M}) = -\lambda (k - m\lambda)(k(2m+M) - mM\lambda) = 0$$

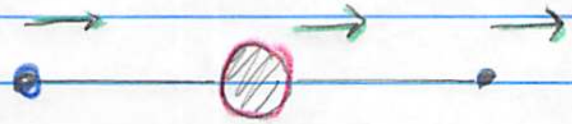
Either way there are three modes:

① $\lambda_0 = 0$ $\qquad \vec{E}_0 = (1, 1, 1)$

② $\lambda_1 = \omega_1^2 = k/m$ $\qquad \vec{E}_1 = (-1, 0, 1)$

③ $\lambda_2 = \omega_2^2 = \frac{k}{m}\left(1 + \frac{2m}{M}\right)$ $\qquad \vec{E}_2 = \left(1, -\frac{2m}{M}, 1\right)$

## Pictures



$\lambda_0 = 0$ a zero mode

This is just a translation of the system as a whole

$\lambda_1 = k/m$

$\lambda_2 = \frac{k}{m}\left(1 + \frac{2m}{M}\right)$

- Note that the non-zero modes are orthogonal to the zero modes as required

$$(\vec{E}_0, M\vec{E}_1) = (1\ 1\ 1)\begin{pmatrix} m & & \\ & M & \\ & & m \end{pmatrix}\begin{pmatrix} 1 \\ -2m/m \\ 1 \end{pmatrix} = 0$$

- Note that any vector $\vec{Y} = (u^1, u^2, u^3)$ which is orthogonal to the zero mode has no net momentum

$$\frac{d}{dt}(\vec{E}_0, M\vec{Y}) = \frac{d}{dt}(1\ 1\ 1)\begin{pmatrix} m & & \\ & M & \\ & & m \end{pmatrix}\begin{pmatrix} u^1 \\ u^2 \\ u^3 \end{pmatrix} = 0$$

$$= m\dot{u}^1 + M\dot{u}^2 + m\dot{u}^3 = 0$$

- Each mode is independent. So a general displacement expanded in the Eigen basis is

$$\vec{X} = (u^1, u^2, u^3)$$

$$= \vec{E}_0 \, X^0(t) + \vec{E}_1 \, X^1(t) + \vec{E}_2 \, X^2(t)$$

- So each amplitude $X^a(t)$ satisfies

$$\boxed{\frac{d^2 X^a}{dt^2} = \omega_a^2 X^a}$$

$X^a = A \cos(\omega_a t + \phi)$

or if $\omega_a = 0$

$X^a = A + Bt$

So the general solution is

$$\boxed{\begin{aligned}\vec{X} = \vec{E}_0 \, (A + Bt) + \vec{E}_1 A_1 \cos(\omega_1 t + \phi_1) \\ + \vec{E}_2 A_2 \cos(\omega_2 t + \phi_2)\end{aligned}}$$