Normal Modes Problem 1

Cartesian coord's of nuclei: x_1, x_2 ; Masses m

$$V(x_1, x_2) \simeq \frac{1}{2} k \left(x_2 - x_1 - a\right)^2 , \qquad a: \text{equilibrium bond length}$$

Mass weighted: $q_1 = \sqrt{m}\, x_1$, $q_2 = \sqrt{m}\, x_2$

$$\frac{\partial^2 V}{\partial x_1^2} = k, \qquad \frac{\partial^2 V}{\partial x_2^2} = k, \qquad \frac{\partial^2 V}{\partial x_1 \partial x_2} = -k$$

$$\tilde{K} = \begin{pmatrix} \frac{k}{m} & -\frac{k}{m} \\ -\frac{k}{m} & \frac{k}{m} \end{pmatrix}$$ has the familiar simple form.

Eigenvalues: $$\frac{k}{m} \pm \left(-\frac{k}{m}\right) = 0 \text{ or } \frac{2k}{m}$$

For eigenvalue 0, eigenvector is $Q_1 = \frac{1}{\sqrt{2}}\left(q_1 + q_2\right) = \frac{\sqrt{m}}{\sqrt{2}}\left(x_1 + x_2\right)$

For eigenvalue $\frac{2k}{m}$, eigenvector is $Q_2 = \frac{1}{\sqrt{2}}\left(q_2 - q_1\right) = \frac{\sqrt{m}}{\sqrt{2}}\left(x_2 - x_1\right)$

In the normal mode coord's the Hamiltonian is

$$\begin{aligned} H &= \frac{1}{2}\dot{Q}_1^2 + \frac{1}{2}\dot{Q}_2^2 + \frac{1}{2}\cdot 0 \cdot Q_1^2 + \frac{1}{2}\cdot\left(\frac{2k}{m}\right)\cdot Q_2^2 \\ &= \frac{1}{2}\cdot\frac{m}{2}\left(\dot{x}_1 + \dot{x}_2\right)^2 + \frac{1}{2}\,\frac{m}{2}\left(\dot{x}_2 - \dot{x}_1\right)^2 + \frac{1}{2}\cdot\frac{2k}{m}\left(\sqrt{\frac{m}{2}}\right)^2\left(x_2 - x_1\right)^2 \end{aligned}$$

With $M = 2m$ (total mass), $\mu = \frac{m}{2}$ (reduced mass), $R = \frac{x_1 + x_2}{2}$, $r = x_2 - x_1$

$$H = \underset{\substack{\uparrow \\ \text{translation}}}{\frac{1}{2} M \dot{R}^2} + \underbrace{\frac{1}{2}\mu \dot{r}^2}_{\text{vibration}} + \frac{1}{2} k r^2$$