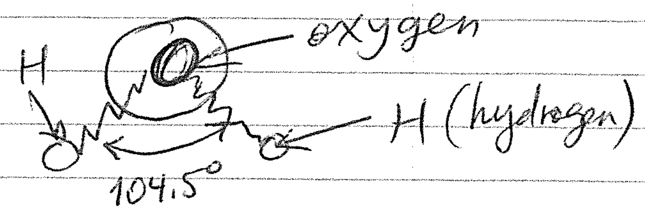
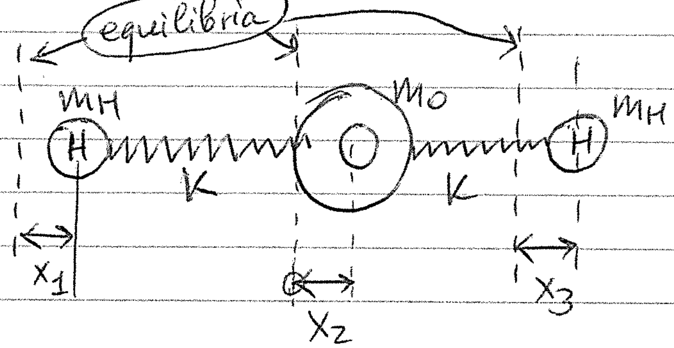
Last lecture in the course:

Application — oscillations of H_2O molecule

H_2O molecule:



Simplified view:



We approximate the restoring force between the O- and H-atoms using Hooke's law

$$F_{spring} = -K \cdot \Delta x$$ change of spring's length.

Use 2nd Law of Newton: $ma = F$ ← acceleration, d^2x/dt^2.

$$m_H \frac{d^2x_1}{dt^2} = -K(x_1 - x_2)$$

$$m_O \frac{d^2x_2}{dt^2} = -K(x_2 - x_1) - K(x_2 - x_3)$$

$$m_H \frac{d^2x_3}{dt^2} = -K(x_3 - x_2)$$

The l.h.s. can be written as matrix · vector:

$$\underbrace{\begin{pmatrix} m_H & & 0 \\ & m_O & \\ 0 & & m_H \end{pmatrix}}_{M,\ \text{symmetric}} \frac{d^2}{dt^2} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_{\underline{x}} = \underbrace{\begin{pmatrix} -k & k & 0 \\ k & -2k & k \\ 0 & k & -k \end{pmatrix}}_{K,\ \text{symmetric.}} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \qquad (1a)$$

Can continue as:

$$\frac{d^2 \underline{x}}{dt^2} = (M^{-1} K) \underline{x}, \qquad (1b)$$

but won't do that.
Reason: $(M^{-1}K)$ is not symmetric (even though M and M^{-1} and K are symmetric, but $M^{-1}K$ is not because M^{-1} & K do not commute:
$A^T = A$, $B^T = B$, but $(AB)^T \neq AB$ since $AB \neq BA$;
we did this in Sec. 1.6).

Although calculations can be done with a non-symmetric $(M^{-1}K)$, they are nicer with a symmetric matrix. Therefore, we proceed differently.

Note: $$M = \begin{pmatrix} m_H & & 0 \\ & m_O & \\ 0 & & m_H \end{pmatrix} = \overbrace{\begin{pmatrix} \sqrt{m_H} & & 0 \\ & \sqrt{m_O} & \\ 0 & & \sqrt{m_H} \end{pmatrix}}^{\sqrt{M}} \overbrace{\begin{pmatrix} \sqrt{m_H} & & 0 \\ & \sqrt{m_O} & \\ 0 & & \sqrt{m_H} \end{pmatrix}}^{\sqrt{M}}.$$

So, $M = \sqrt{M} \cdot \sqrt{M}$.

Note that $\sqrt{M}$ is also symmetric:

$$\sqrt{M}^{T} = \sqrt{M} \qquad (2)$$

Now, transform (1b) as follows:

$$\sqrt{M}\,\sqrt{M}\,\frac{d^2 \underline{x}}{dt^2} = K \sqrt{M}^{-1}\sqrt{M}\,\underline{x} \quad \Rightarrow$$

$$\frac{d^2}{dt^2}\underbrace{(\sqrt{M}\,\underline{x})}_{\underline{y}} = \underbrace{\left(\sqrt{M}^{-1} K \sqrt{M}^{-1}\right)}_{A}(\sqrt{M}\,\underline{x}) \qquad (3a)$$

$$\frac{d^2 \underline{y}}{dt^2} = A\,\underline{y}, \qquad (3b)$$

where now A is symmetric. Indeed:

$$A^{T} = \left(\sqrt{M}^{-1} K \sqrt{M}^{-1}\right)^{T} = \left(\sqrt{M}^{-1}\right)^{T} K^{T} \left(\sqrt{M}^{-1}\right)^{T}$$

$\sqrt{M}^{-1}$ and K are symmetric

$$\overset{\downarrow}{=} \sqrt{M}^{-1} K \sqrt{M}^{-1} = A. \quad \checkmark$$

Now let's find its explicit form:

$$A = \begin{pmatrix} \frac{1}{\sqrt{m_H}} & & 0 \\ & \frac{1}{\sqrt{m_O}} & \\ 0 & & \frac{1}{\sqrt{m_H}} \end{pmatrix} \begin{pmatrix} -k & k & 0 \\ k & -2k & k \\ 0 & k & -k \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{m_H}} & & 0 \\ & \frac{1}{\sqrt{m_O}} & \\ 0 & & \frac{1}{\sqrt{m_H}} \end{pmatrix} =$$

App-4

$$= \begin{pmatrix} -\frac{k}{m_H} & \frac{k}{\sqrt{m_H m_O}} & 0 \\ \frac{k}{\sqrt{m_H m_O}} & -\frac{2k}{m_O} & \frac{k}{\sqrt{m_H m_O}} \\ 0 & \frac{k}{\sqrt{m_H m_O}} & -\frac{k}{m_H} \end{pmatrix} \overset{\text{notation}}{\equiv} \underbrace{\begin{pmatrix} -a & b & 0 \\ b & -2c & b \\ 0 & b & -a \end{pmatrix}}_{A}$$

Note:

$$ac = b^2 \qquad (4)$$

$$\left(\frac{k}{m_H} \cdot \frac{k}{m_O} = \left(\frac{k}{\sqrt{m_H m_O}} \right)^2 \right)$$

We now seek solution of (3b) in the form: (App-3)

$$\underline{y}(t) = e^{\sqrt{\lambda} t} \, \underline{u} \leftarrow \text{independent of } t. \qquad (5)$$

Substitute (5) into (3b):

$$(\sqrt{\lambda})^2 \cancel{e^{\sqrt{\lambda} t}} \, \underline{u} = A \cancel{e^{\sqrt{\lambda} t}} \, \underline{u} \quad \Rightarrow$$

$$A \underline{u} = \lambda \underline{u} \qquad (6)$$

the eigenvalue problem!

Its eigenvalues and eigenvectors are found ~~by~~ as usual (with some effort, but straightforwardly):

$$\lambda_1 = -a, \quad \underline{u}_1 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

$$\lambda_2 = 0, \quad \underline{u}_2 = \begin{pmatrix} 1 \\ a/b \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ \sqrt{m_O/m_H} \\ 1 \end{pmatrix} \qquad (7)$$

$$\lambda_3 = -(2c+a), \quad \underline{u}_3 = \begin{pmatrix} 1 \\ -2b/a \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -2\sqrt{m_H/m_O} \\ 1 \end{pmatrix}$$

As the general theory predicts, they are all orthogonal.

Returning to Eq. (5) on p. App-4, we see that we have found 3 solutions of the diff. equation (36) (p. App-3):

$$y_1 = e^{\sqrt{\lambda_1}\,t}\,\underline{u}_1, \quad y_2 = e^{\sqrt{\lambda_2}\,t}\,\underline{u}_2, \quad y_3 = e^{\sqrt{\lambda_3}\,t}\,\underline{u}_3.$$

How do we use them to construct the general solution of the diff. eq. and also its solution with a particular initial condition?

We use the fact that the diff. eq. (36) is linear and homogeneous. Then its solutions form a linear vector space (Sec. 3.2). This means that any linear combination of solutions is also a solution of (36)!

So the most general solution of (36) is:

$$\underline{y}(t) = c_1 e^{\sqrt{\lambda_1}t}\underline{u}_1 + c_2 e^{\sqrt{\lambda_2}t}\underline{u}_2 + c_3 e^{\sqrt{\lambda_3}t}\underline{u}_3 \qquad (8)$$

(simplification: we dropped terms $e^{-\sqrt{\lambda_1}t}\underline{u}_1$ etc.)

How do we find c_1, c_2, c_3?
From the initial condition!

$$\underline{y}(0) = c_1 \cdot \cancelto{1}{e^{\sqrt{\lambda_1}0}}\,\underline{u}_1 + c_2\underline{u}_2 + c_3\underline{u}_3 . \qquad (9)$$

↑ known i.c.

(Note: This is a simplification (see note after (8)), but the basic idea is correct.)

Since $\underline{u}_1, \underline{u}_2, \underline{u}_3$ are orthogonal, the coordinates c_1, c_2, c_3 are found easily:

$$c_j = \frac{\underline{u}_j^T\,\underline{y}(0)}{\underline{u}_j^T\,\underline{u}_j} \qquad (10)$$

Thus, $\underline{y}(t) = \sqrt{M}\,\underline{x}(t)$ has been found.

Let us now write the answer in terms of $\underline{x}$ and interprete it.

$$\underline{y} = \sqrt{M}\,\underline{x} \quad \Rightarrow \quad \underline{u} = \sqrt{M}\,\underline{v} \rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\Rightarrow \quad \underline{v}_j = \sqrt{M}^{-1}\,\underline{u}_j .$$

1 $$\underline{u}_1 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \quad \underline{v}_1 = \begin{pmatrix} 1/\sqrt{m_H} & & 0 \\ & 1/\sqrt{m_O} & \\ 0 & & 1/\sqrt{m_H} \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \Rightarrow$$

$$\Rightarrow \quad \underline{v}_1 = \begin{pmatrix} -1/\sqrt{m_H} \\ 0 \\ 1/\sqrt{m_H} \end{pmatrix} \sim \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} .$$

2 $$\underline{u}_2 = \begin{pmatrix} 1 \\ \sqrt{m_O/m_H} \\ 1 \end{pmatrix} \Rightarrow \quad \underline{v}_2 = \begin{pmatrix} 1/\sqrt{m_H} & & 0 \\ & 1/\sqrt{m_O} & \\ 0 & & 1/\sqrt{m_H} \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{m_O/m_H} \\ 1 \end{pmatrix}$$

$$\underline{v}_2 = \begin{pmatrix} 1/\sqrt{m_H} \\ 1/\sqrt{m_H} \\ 1/\sqrt{m_H} \end{pmatrix} \sim \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} .$$

3 $$\underline{u}_3 = \begin{pmatrix} 1 \\ -2\sqrt{m_H/m_O} \\ 1 \end{pmatrix} \Rightarrow \quad \underline{v}_3 = \ldots \begin{pmatrix} 1/\sqrt{m_H} \\ -2\sqrt{m_H}/m_O \\ 1/\sqrt{m_H} \end{pmatrix} \sim \begin{pmatrix} 1 \\ -2\frac{m_H}{m_O} \\ 1 \end{pmatrix} .$$

$$m_O / m_H \approx 16/1, \Rightarrow \underline{v}_3 = \begin{pmatrix} 1 \\ -1/8 \\ 1 \end{pmatrix} .$$

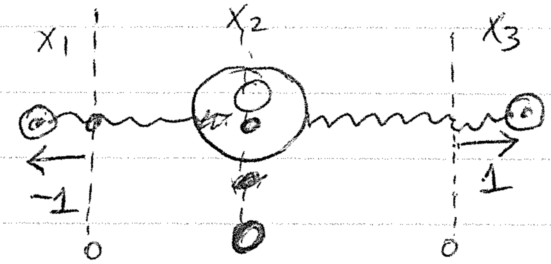
So

$$\underline{X}(t) = c_1 e^{\underbrace{\sqrt{-a}}_{\sqrt{-\frac{k}{m_H}} = i\sqrt{\frac{k}{m_H}}}\,t} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} + c_2 e^{at} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + c_3 e^{\sqrt{-(2b+a)}\,t} \begin{pmatrix} 1 \\ -1/8 \\ 1 \end{pmatrix} \qquad (11)$$

$$e^{i\alpha t} = \cos(\alpha t) + i \cdot \sin(\alpha t) \leftarrow \text{oscillations.}$$

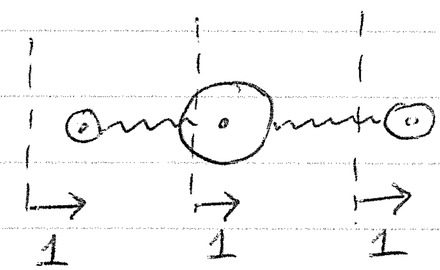
Interpretation:

$\underline{v}_1 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$



Center remains fixed.

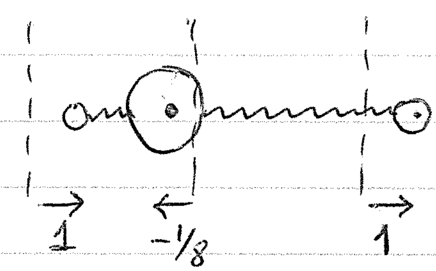
$\underline{v}_2 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$



This is simply a translation!

This is why its time dependence is $\sim e^{0 \cdot t}$ (time independent!) — no oscillations.

$\underline{v}_3 = \begin{pmatrix} 1 \\ -1/8 \\ 1 \end{pmatrix}$



Asymmetric oscillation.

Thus: The motion of a 3-atomic molecule is a linear combination of 2 oscillatory modes ($\underline{v}_1$, $\underline{v}_3$) and 1 translation ($\underline{v}_2$).