Recall:

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{x} = \mathbf{A}\vec{x} \qquad \text{with } \mathbf{A} \text{ an } n \times n \text{ matrix}$$

We can find n solutions $\vec{x}(t) = e^{\lambda t}\vec{v}$ by finding the eigenvalues, λ, and eigenvectors, $\vec{v}$, of the matrix $\mathbf{A}$.

i.e., solving

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \quad \text{and} \quad (\mathbf{A} - \lambda\mathbf{I})\vec{v} = 0$$

What about if we have $\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x} = \mathbf{A}\vec{x}$?

Could convert to a larger 1st order system...but lets try something else.

Simple second order systems

Suppose we want to find the general solution to

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x} = \mathbf{A}\vec{x}$$

Lets guess $\vec{x}(t) = e^{rt}\vec{v}$

$$r^2 e^{rt}\vec{v} = \mathbf{A}e^{rt}\vec{v}$$

$$r^2\vec{v} = \mathbf{A}\vec{v} \qquad \Rightarrow \lambda = r^2 \text{ is an eigenvalue of } \mathbf{A}$$

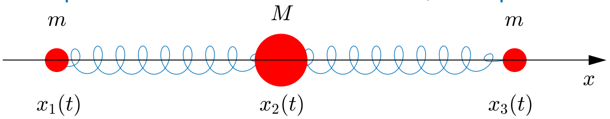
For matrices with real entries, 2 cases:

1. $r^2 > 0 \quad \Rightarrow \quad \vec{x}_\lambda(t) = \left(c_1 e^{\sqrt{\lambda}t} + c_2 e^{-\sqrt{\lambda}t}\right)\vec{v}$
2. $r^2 < 0$

$$\begin{aligned}\Rightarrow \quad \vec{x}_\lambda(t) &= \left(d_1 e^{i\sqrt{|\lambda|}t} + d_2 e^{-i\sqrt{|\lambda|}t}\right)\vec{v}\\ &= \left(c_1\cos(\sqrt{|\lambda|}t) + c_2\sin(\sqrt{|\lambda|}t)\right)\vec{v}\end{aligned}$$

Linear model of H_2O

Consider a linear representation of a water molecule, as depicted below.



Let x_1 and x_3 be the displacement of the hydrogen atoms from their equilibrium positions, and x_2 be the displacment of the oxygen molecule.

Treat the atoms as if they are connected by springs with stiffness k.

From Newton's 2nd law:

$$\begin{aligned} mx_1'' &= k(x_2 - x_1) \\ Mx_2'' &= k(x_3 - x_2) - k(x_2 - x_1) \\ mx_3'' &= -k(x_3 - x_2) \end{aligned}$$

Let $\vec{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$

Then we have

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x} = \omega_0^2 \begin{bmatrix} -1 & 1 & 0 \\ \alpha & -2\alpha & \alpha \\ 0 & 1 & -1 \end{bmatrix} \vec{x}$$

$$w_0 = \sqrt{k/m} \qquad \alpha = m/M$$

The eigensolutions of our water model

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x} = \mathbf{A}\vec{x}, \qquad \mathbf{A} = \omega_0^2 \begin{bmatrix} -1 & 1 & 0 \\ \alpha & -2\alpha & \alpha \\ 0 & 1 & -1 \end{bmatrix}$$

$$w_0 = \sqrt{k/m}$$
$$\alpha = m/M$$

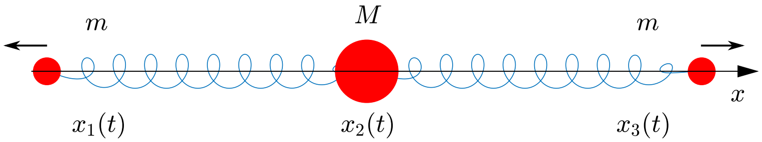
$$\lambda_1 = -\omega_0^2 \qquad \vec{v}_1 = \begin{bmatrix} -1 & 0 & 1 \end{bmatrix}^T$$
$$\vec{x}_1 = (c_1 \cos(\omega_0 t) + c_2 \sin(\omega_0 t))\,\vec{v}_1$$

$$\lambda_2 = 0 \qquad \vec{v}_2 = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T$$
$$\vec{x}_2 = (c_3 + c_4 t)\vec{v}_2$$

$$\lambda_3 = -(1+2\alpha)\omega_0^2 \qquad \vec{v}_3 = \begin{bmatrix} 1 & -2\alpha & 1 \end{bmatrix}^T$$
$$\vec{x}_3 = \left(c_4 \cos(\sqrt{1+2\alpha}\,\omega_0 t) + c_5 \sin(\sqrt{1+2\alpha}\,\omega_0 t)\right)\vec{v}_3$$

Eigenmode 1 ($\lambda = -\omega_0^2$)

$$\vec{x}_1 = (c_1 \cos(\omega_0 t) + c_2 \sin(\omega_0 t)) \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$



An oscillation with angular frequency ω_0 where the middle atom remains fixed, and the outer atoms move in opposite directions.

Eigenmode 2 ($\lambda = 0$)

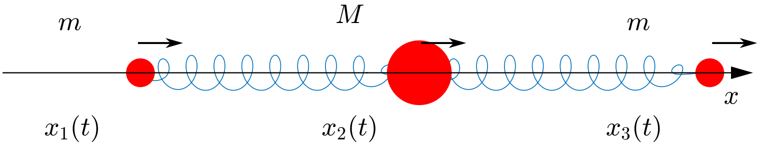
$$\vec{x}_2 = (c_3 + c_4 t) \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Suppose $\vec{x}_2 = T(t)\vec{v}_2$

$$\frac{d^2}{dt^2}\vec{x}_2 = \mathbf{A}\vec{x}_2 = \lambda\vec{x}_2 = \vec{0} = T''\vec{v}_2$$

$$T'' = 0$$

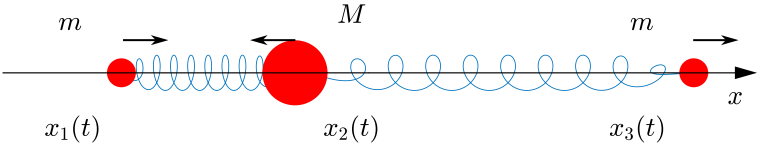
$\Rightarrow T(t) =$ linear function



A translation of the whole molecule.

Eigenmode 3 ($\lambda = -(1+2\alpha)\omega_0^2$)

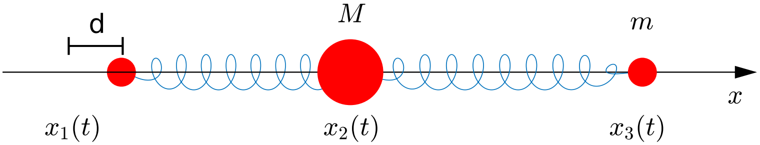
$$\vec{x}_3 = \left(c_4 \cos(\sqrt{1+2\alpha}\,\omega_0 t) + c_5 \sin(\sqrt{1+2\alpha}\,\omega_0 t)\right) \begin{bmatrix} 1 \\ -2\alpha \\ 1 \end{bmatrix}$$



An oscillation with angular frequency $\sqrt{1+2\alpha}\,\omega_0$ where the middle atom moves in the opposite directions as the two outer atoms.

A perturbation

Suppose we displace the leftmost hydrogen a distance d and release it with zero velocity.



That is, $\vec{x}(0) = \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix}$ and $\vec{x}'(0) = \vec{0}$

How will the system react? - [Desmos Demo]

Notes:

The equations of motion of each atom can be decomposed into contributions from the three eigenmodes.

How much each mode contributes is entirely determined by the initial conditions.

Now with forcing...

Suppose that instead of moving the hydrogen atom, we apply a periodic force to it.

$$\frac{d^2}{dt^2}\vec{x} = \mathbf{A}\vec{x} + \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix} \sin(\Omega t)$$

Method of undetermined coefficients

$$\vec{x}_p = \cancelto{\vec{0}}{\vec{f}} \cos(\Omega t) + \vec{g} \sin(\Omega t)$$

This assumes we have no resonance, i.e.

$$\Omega \neq \omega_0, 0, \sqrt{1 + 2\alpha}\omega_0$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x}_p = \mathbf{A}\vec{x}_p + \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix} \sin(\Omega t)$$

$$\vec{x}_p = \vec{g}\sin(\Omega t) \qquad \Rightarrow \frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x}_p = -\Omega^2 \sin(\Omega t)\vec{g}$$

$$-\Omega^2 \sin(\Omega t)\vec{g} = \mathbf{A}\vec{g}\sin(\Omega t) + \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix} \sin(\Omega t)$$

$$-(\mathbf{A} + \Omega^2 \mathbf{I})\vec{g} = \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix}$$

$$\vec{g} = -(\mathbf{A} + \Omega^2 \mathbf{I})^{-1} \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix}$$

Resonance

$$\vec{x}(t) = \vec{x}_h(t) - (\mathbf{A} + \Omega^2 \mathbf{I})^{-1} \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix} \sin(\Omega t)$$

Does the matrix $(\mathbf{A} + \Omega^2 \mathbf{I})^{-1}$ always exist?

No, not when $-\Omega^2$ is an eigenvalue of $\mathbf{A}$.

Recall, to find the eigenvalue λ:

$$\det(\mathbf{A} - \lambda \mathbf{I}) = 0$$

Since, a matrix inverse has the $1/det$ in it, the matrix inverse would not exist.

This corresponds to resonance.

Resonance Demo

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x} = \omega_0^2 \begin{bmatrix} -1 & 1 & 0 \\ \alpha & -2\alpha & \alpha \\ 0 & 1 & -1 \end{bmatrix} \vec{x} + \begin{bmatrix} d \\ 0 \\ 0 \end{bmatrix} \sin(\Omega t) \qquad \begin{matrix} w_0 = \sqrt{k/m} \\ \alpha = m/M \end{matrix}$$

With $\alpha = 0.5$, $\omega_0 = 0.1$ we have resonances at

$$\begin{aligned} \Omega = \sqrt{-\lambda} &= \omega_0,\ 0, \sqrt{1+2\alpha}\omega_0 \\ &= 0.1,\ 0,\ 0.141421 \end{aligned}$$

[Desmos Demo]