

Systems of ODEs

The ODEs:

$$\begin{aligned}\ddot{x}_1 &= \omega^2(x_2 - x_1 - b) \\ \ddot{x}_2 &= \Omega^2(x_3 - 2x_2 + x_1) \\ \ddot{x}_3 &= \omega^2(x_2 - x_3 + b)\end{aligned}$$

If we insert $x_1 = 0$, $x_2 = b$ and $x_3 = 2b$ into the right-hand sides of the ODEs, we find that $\ddot{x}_1 = \ddot{x}_2 = \ddot{x}_3 = 0$, implying the molecules, if started at these points, remains there. That is, $(0, b, 2b)$ is a position of equilibrium.

Now let $x_1 = y_1$, $x_2 = b + y_2$ and $x_3 = 2b + y_3$. The ODEs become

$$\begin{aligned}\ddot{y}_1 &= \omega^2(y_2 - y_1) \\ \ddot{y}_2 &= \Omega^2(y_3 - 2y_2 + y_1) \\ \ddot{y}_3 &= \omega^2(y_2 - y_3)\end{aligned}$$

which can be placed into the matrix form as required.

Now let $\mathbf{y} = \mathbf{y}_0 e^{i\nu t}$. We find the linear system, $(A + \nu^2 I)\mathbf{y}_0 = \mathbf{0}$. The characteristic frequencies follow from zero-ing the determinant,

$$\begin{vmatrix} \nu^2 - \omega^2 & \omega^2 & 0 \\ \Omega^2 & \nu^2 - 2\Omega^2 & \Omega^2 \\ 0 & \omega^2 & \nu^2 - \omega^2 \end{vmatrix} = 0$$

Expanding, we find

$$\nu^2(\nu^2 - \omega^2)(\nu^2 - \omega^2 - 2\Omega^2) = 0.$$

The characteristic frequencies are therefore $\nu = 0, \pm\omega$ and $\pm\sqrt{\omega^2 + 2\Omega^2}$.

The eigenvectors associated with these frequencies are

$$A \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad B \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad C \begin{pmatrix} \omega^2 \\ -2\Omega^2 \\ \omega^2 \end{pmatrix},$$

where A, B and C are arbitrary constants.

The general solution is therefore

$$\mathbf{y} = (A_1 + B_1 t) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + (A_2 e^{i\omega t} + B_2 e^{-i\omega t}) \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + (A_3 e^{i\nu_3 t} + B_3 e^{-i\nu_3 t}) \begin{pmatrix} \omega^2 \\ -2\Omega^2 \\ \omega^2 \end{pmatrix},$$

where $\nu_3 = \sqrt{\omega^2 + 2\Omega^2}$, and A_j and B_j , for $j = 1, 2$ and 3 , are arbitrary constants. Note that, in the first term we must add a second solution, $B_1 t$, in order to complete that pair of solutions.

The first part of the solution (normal mode) contains two parts: A_1 is a constant displacement of the molecule; $B_1 t$ is a steady drift of the molecule. Each atom is either displaced by the same amount, or the molecule drifts as a fixed unit without stretching either of the bonds.

The second mode is an oscillation with frequency ω . The middle atom remains stationary, whilst the outer two atoms oscillate perfectly out of phase.

The third mode is an oscillation with frequency $\nu_3 = \sqrt{\omega^2 + 2\Omega^2}$. The outer atoms oscillate perfectly in phase; the middle atom is now out of phase, and oscillates with a different amplitude.

With the source of photons, the system of ODEs has an added, periodic forcing term. The molecular vibrations then pick up a forced response, described by a particular solution of the form $\mathbf{v} \cos \mu t$, where $\mathbf{v} = -(A + \mu^2 I)^{-1} \mathbf{f}$. This solution exists provided μ^2 is distinct from either of the characteristic values $0, \omega^2$ or $\omega^2 + 2\Omega^2$. If μ^2 takes one of these values, resonance occurs and growing oscillations result. Nearby these frequencies, beats can be observable, in the form of strong intermittent molecular vibrations that wax and wane on a long timescale.

Laplace transforms

- (a) $2/(s-4)$. (b) $4/s^3 - 1/(s+1)$. (c) $3s/(s^2+25)$. (d) $3(s^2-36)/(s^2+36)^2$. (e) $60/[(s-3)^2+36]$.
- (a) $e^{-2t}/2$. (b) te^{3t} . (c) $1 - e^{-at}$. (d) $1 - \cos kt$. (e) $6e^{2t} \cos 4t + 2e^{2t} \sin 4t$.
- (a) transforming the ODE leads to

$$\bar{y} = \frac{1}{(s-a)^2 + b^2}.$$

Thence,

$$y = \frac{1}{b} e^{at} \sin bt.$$

For (b),

$$\bar{y} = \frac{1}{(s^2+4)(s^2+1)} = \frac{1}{3(s^2+1)} - \frac{1}{3(s^2+4)},$$

using a partial fraction. Then,

$$y = \frac{1}{3} \sin t - \frac{1}{6} \sin 2t$$

For (c), we find

$$\bar{y} = \bar{z} + \frac{1}{s^2}, \quad \bar{z} = -\frac{(s^2+1)}{s^2(s+1)^2}.$$

Using partial fractions:

$$\bar{z} = \frac{2}{s} - \frac{1}{s^2} - \frac{2}{s+1} - \frac{2}{(s+1)^2}, \quad \bar{y} = \frac{2}{s} - \frac{2}{s+1} - \frac{2}{(s+1)^2}.$$

Thus,

$$z = 2 - t - 2e^{-t} - 2te^{-t}, \quad y = 2 - 2e^{-t} - 2te^{-t}.$$