Assignment 5 - PHYS 331

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April 9th 2024

1 Coupled masses

1.1 Part a)

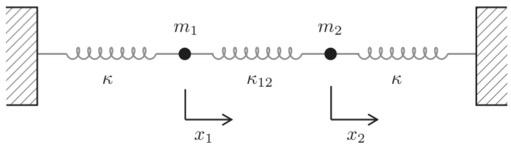


Figure 34: coupled oscillators

Consider a system of coupled oscillators with masses m_1 and m_2, connected by the springs with spring constants κ and κ_{12}. Let x_1 and x_2 represent the displacements from equilibrium for the first and second masses, respectively. The total potential energy of the system can be expressed as:

$$V(x_1, x_2) = \frac{1}{2}\kappa x_1^2 + \frac{1}{2}\kappa_{12}(x_2 - x_1)^2 + \frac{1}{2}\kappa x_2^2$$

$$V(x_1, x_2) = \frac{1}{2}(\kappa + \kappa_{12})x_1^2 + \frac{1}{2}(\kappa + \kappa_{12})x_2^2 - \kappa_{12}x_1 x_2$$

Then we can calculate matrix elements:

$$A_{11} = \left.\frac{\partial^2 V}{\partial x_1^2}\right|_{x_1=0} = \kappa + \kappa_{12}$$

$$A_{12} = A_{21} = \left.\frac{\partial^2 V}{\partial x_1 \partial x_2}\right|_{x_1=x_2=0} = -\kappa_{12}$$

$$A_{22} = \left.\frac{\partial^2 V}{\partial x_2^2}\right|_{x_2=0} = \kappa + \kappa_{12}$$

And construct the matrix A as:

$$A = \begin{pmatrix} \kappa + \kappa_{12} & -\kappa_{12} \\ -\kappa_{12} & \kappa + \kappa_{12} \end{pmatrix}$$

Then we can calculate the kinetic energy as

$$T(x_1, x_2) = \frac{1}{2}M(\dot{x}_1^2 + \dot{x}_2^2)$$

We define the matrix M to be diagonal with the elements m_{ij} as follows:

$$m_{11} = m_1 = M$$

$$m_{22} = m_2 = M$$

$$m_{12} = m_{21} = 0$$

We obtain

$$M = \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}$$

Next, we need to solve $\det(A - \omega^2 M) = 0$.

$$\begin{pmatrix} \kappa + \kappa_{12} - M\omega^2 & -\kappa_{12} \\ -\kappa_{12} & \kappa + \kappa_{12} - M\omega^2 \end{pmatrix} = 0$$

$$(\kappa + \kappa_{12} - M\omega^2)^2 - (\kappa_{12}^2) = 0$$

Which has roots of the form

$$\omega^2 = \frac{\kappa + \kappa_{12} \pm \kappa_{12}}{M}$$

Which yields two solutions

$$\omega_1^2 = \frac{\kappa + 2\kappa_{12}}{M} \qquad \text{and} \qquad \omega_2^2 = \frac{\kappa}{M}$$

By plugging each of those solutions in our calculated determinant yields the following relations, respectively

$$a_{11} = -a_{21} \qquad \text{and} \qquad a_{12} = a_{22}$$

And we can define our eigenmodes as

$$x_1 = a_{11}\phi_1 + a_{22}\phi_2 \qquad \text{and} \qquad x_2 = -a_{11}\phi_1 + a_{22}\phi_2$$

with the normal basis defined as

$$\phi_2 = \frac{1}{2a_{11}}(x_1 + x_2) \qquad \text{and} \qquad \phi_1 = \frac{1}{2a_{22}}(x_1 - x_2)$$

1.2 Part b)

The most general solution is the eigenmodes given above which can be restated here

$$x_1 = a_{11}\phi_1 + a_{22}\phi_2 \qquad \text{and} \qquad x_2 = -a_{11}\phi_1 + a_{22}\phi_2$$

1.3 Part c)

Recall our normal basis

$$\phi_2 = \frac{1}{2a_{11}}(x_1 + x_2) \qquad \text{and} \qquad \phi_1 = \frac{1}{2a_{22}}(x_1 - x_2)$$

We observe that when $x_1 = x_2$, $\phi_1 = 0$ and the system oscillates in-phase at ω_2 since that oscillation only depends on κ. On the other hand, when x_1 = -x_2 the oscillation is out-of-phase since the only non-zero normal mode is ϕ_1 which oscillates at ω_1 which depends on both κ and κ_{12}.

1.4 Part d)

The new matrix will be

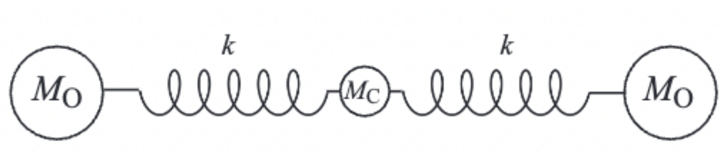
$$\begin{pmatrix} \kappa + \kappa_{12} - m_1\omega^2 & -\kappa_{12} \\ -\kappa_{12} & \kappa + \kappa_{12} - m_2\omega^2 \end{pmatrix} = 0$$

$$(\kappa + \kappa_{12} - m_1\omega^2)(\kappa + \kappa_{12} - m_2\omega^2) - (\kappa_{12}^2) = 0$$

And the roots are now

$$\Omega = \frac{(\kappa_{12} + \kappa)(m_1 + m_2) \pm \sqrt{(\kappa_{12} + \kappa)^2(m_1 + m_2)^2 - 4\kappa(m_1 m_2)(\kappa + 2\kappa_{12})}}{2m_1 m_2}$$

2 Carbon Dioxide molecule



2.1 Part a)

We define the kinetic energy as

$$T = \frac{1}{2}M_o\dot{x_1}^2 + \frac{1}{2}M_c\dot{x_2}^2 + \frac{1}{2}M_0\dot{x_3}^2$$

The potential energy of of the springs arises from the relative displacement of adjacent atoms

$$V = \frac{1}{2}k(x_2 - x_1)^2 + \frac{1}{2}k(x_3 - x_2)^2$$

We have everything to compute the Lagrangian

$$\mathcal{L} = T - V = \frac{1}{2}M_o\dot{x_1}^2 + \frac{1}{2}M_c\dot{x_2}^2 + \frac{1}{2}M_0\dot{x_3}^2 - \frac{1}{2}k(x_2 - x_1)^2 - \frac{1}{2}k(x_3 - x_2)^2$$

2.2 Part b)

We construct the A matrix as

$$A = \begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix}$$

The matrix M is defined as follows

$$M = \begin{bmatrix} M_o & 0 & 0 \\ 0 & M_c & 0 \\ 0 & 0 & M_o \end{bmatrix}$$

We are left to do an eigenvalue problem defined as $\det(A - \omega^2 M) = 0$. We find 3 eigenvalues

$$\omega_1^2 = 0 \qquad \omega_2^2 = \frac{k}{M_o} \qquad \omega_3^2 = \frac{k(2M_o + M_c)}{M_o M_c}$$

2.3 Part c)

We have $\omega_1 = 0$ so as indicated, I won't proceed to find the eigenvector v. For the other frequencies, we will determine the relative displacements $x_1 : x_2 : x_3$. Let's start with ω_2,

$$0 = \begin{bmatrix} 0 & -k & 0 \\ -k & \frac{k(2M_o - M_c)}{M_o} & -k \\ 0 & -k & 0 \end{bmatrix} v$$

Which yields $x_2 = 0$ and $x_1 = -x_3$. Therefore, the relative displacements are $1 : 0 : -1$ for that mode. Next, we proceed for ω_3,

$$0 = \begin{bmatrix} \frac{-2kM_o}{M_c} & -k & 0 \\ -k & \frac{-kM_c}{M_o} & -k \\ 0 & -k & \frac{-2kM_o}{M_c} \end{bmatrix} v$$

We obtain the relations $x_1 = x_3$ and $x_1 = \frac{-M_c}{2M_o} x_2$ and the relative displacements $1 : \frac{-M_c}{2M_o} : 1$ for this mode.