

1 Topic 6: Coupled Oscillators and Normal Modes

Reading assignment: Hand and Finch Chapter 9

We are going to be considering the general case of a system with N degrees of freedom close to one of its stable equilibrium points. We are going to show that for small displacements from equilibrium, the system acts like N independent SHOs, usually with N different characteristic frequencies. One or more of these SHOs can be excited, depending on the initial conditions. If only one oscillation frequency is excited, the N degrees of freedom move synchronously at a *common mode frequency*. The ratios of the displacements for the different degrees of freedom, known as *mode displacement ratios* are an intrinsic characteristic of the normal mode that is oscillating. Any motion can be described as a linear combination of modes. We will now develop this formally.

1.1 The Double Pendulum Revisited

Recall our solution for the double pendulum. The Lagrangian for this system is:

$$L = \frac{1}{2}ml^2 \left[2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\cos(\theta_1 - \theta_2)\dot{\theta}_1\dot{\theta}_2 \right] + mgl(2\cos\theta_1 + \cos\theta_2)$$

From this, by considering small displacements (throwing out high order terms and making small angle approximations) we got two coupled differential equations:

$$\begin{aligned} 2\ddot{\theta}_1 + \ddot{\theta}_2 &= -2\omega_o^2\theta_1 \\ \ddot{\theta}_1 + \ddot{\theta}_2 &= -g\omega_o^2\theta_2 \end{aligned}$$

We looked explicitly for solutions where both masses oscillate with the same frequency:

$$\theta_{1,2}(t) = \theta_{1,2}e^{\pm i\omega t}$$

Note that we did not find a general solution to the problem – where the oscillations of θ_1, θ_2 are not necessarily at the same frequency.

By substituting our solution into the EOM, we found two linear equations

$$\begin{aligned} 2(\omega_o^2 - \omega^2)\theta_1 - \omega^2\theta_2 &= 0 \\ -\omega^2\theta_1 + (\omega_o^2 - \omega^2)\theta_2 &= 0 \end{aligned}$$

which can have non-trivial solutions only if the determinant of the coefficients vanishes. So, we got two roots corresponding to two different frequencies:

$$\begin{bmatrix} 2(\omega_o^2 - \omega^2) & -\omega^2 \\ -\omega^2 & (\omega_o^2 - \omega^2) \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = 0$$

The determinant vanishing gives us:

$$2(\omega_o^2 - \omega^2)^2 - \omega^4 = 0$$

$$\omega^4 - 4\omega_o^2\omega^2 + 2\omega_o^4 = 0$$

$$\omega_{\pm}^2 = \left[2 \pm \sqrt{2} \right] \omega_o^2$$

And back-substituting into the linear equations gave us the ratios of the amplitudes of oscillation: $\frac{\theta_1}{\theta_2}$.

$$\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = A_1 \begin{bmatrix} 1 \\ -\sqrt{2} \end{bmatrix} e^{i\omega_+ t}$$

$$\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = A_2 \begin{bmatrix} 1 \\ \sqrt{2} \end{bmatrix} e^{i\omega_- t}$$

We are now going to develop this more formally for arbitrary systems with N generalized co-ordinates.

1.2 A Review of Matrix Algebra

The formalism we are about to develop requires some matrix algebra, so lets do a quick review. A collection of basic facts:

Matrix multiplication is not commutative: if we consider two matrices \mathbf{A} and \mathbf{B} :

$$\mathbf{C} = \mathbf{AB} \neq \mathbf{BA}$$

We will use *Einstein summation notation*. In this convention, repeated indices are summed over. So, we would write the product of two matrices as:

$$c_{ij} = a_{ik}b_{kj}$$

where k is summed over, and c_{ij} refers to the ij^{th} element of the matrix \mathbf{C} .

The *transpose* of a matrix is defined by interchanging rows and columns. We write it as

$$\tilde{\mathbf{A}}$$

The *inverse* of a matrix is defined such that if

$$\vec{x}' = \mathbf{A}\vec{x}$$

then

$$\mathbf{A}^{-1}\vec{x}' = \vec{x}$$

so we can easily see that

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{AA}^{-1} = \bar{\mathbf{1}}$$

where $\bar{\mathbf{1}}$ is the identity matrix $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. In the particular case where $\mathbf{A}^{-1} = \tilde{\mathbf{A}}$, then the matrix is said to be *orthogonal*.

The *adjoint* is formed by taking the complex conjugate of $\tilde{\mathbf{A}}$

$$\mathbf{A}^\dagger = \left(\tilde{\mathbf{A}} \right)^*$$

A *unitary* matrix is defined as one where

$$\mathbf{A}^\dagger \mathbf{A} = \mathbf{1}$$

and further, if $\mathbf{A}^\dagger = \mathbf{A}$, the matrix is *self-adjoint* or *hermitian*.

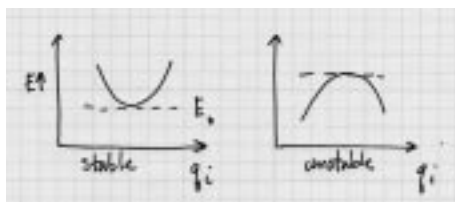
1.3 Small Oscillations

Now return to the problem at hand. Consider a conservative system – no explicit time dependence to L , and $V = V(q)$. We will be looking at systems with small displacements from equilibrium, so that we can linearize the EOM (as we discussed in the last topic). As we saw from expanding the Lagrangian, Taylor's theorem guarantees that most systems are linear if displacements are small enough.

Our condition for static equilibrium states that the generalized forces vanish:

$$Q_i = \left(\frac{\partial V}{\partial q_i} \right)_o = 0$$

This must be true for all dimensions (no saddle points).



In general we can write the Lagrangian as:

$$L = \frac{1}{2} \sum m_{ij}(\vec{q}) \dot{q}_i \dot{q}_j - V(\vec{q})$$

Why does the mass term depend on q ? This will be the case if the co-ordinates are not Cartesian. Take the case of the double pendulum. Here we had the term $2 \cos(\theta_1 - \theta_2) \dot{\theta}_1 \dot{\theta}_2$, so we have a coefficient that depends on the q 's. Our stability condition is:

$$\frac{\partial V}{\partial \vec{q}} = 0$$

If we change co-ordinates in a singular manner: $\vec{q} \rightarrow \vec{q}'$

$$\frac{\partial V}{\partial \vec{q}'} = \frac{\partial V}{\partial \vec{q}} \frac{\partial \vec{q}}{\partial \vec{q}'} = 0$$

implying the static solution is co-ordinate independent.

Lets look at small perturbations about the equilibrium position:

$$\vec{q} \rightarrow \vec{q}_o + \vec{\eta}(t)$$

Expand the potential about the equilibrium position, \vec{q}_o

$$V(\vec{q}) = V(\vec{q}_o) + \left(\frac{\partial V}{\partial \vec{q}} \right)_o \vec{\eta} + \frac{1}{2} \left(\frac{\partial^2 V}{\partial q_i \partial q_j} \right)_o \eta_i \eta_j + h.o.t.$$

The kinetic energy

$$T = \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij} \dot{\eta}_i \dot{\eta}_j$$

Expand the m_{ij}

$$m_{ij}(\vec{q}) = m_{ij}(\vec{q}_o) + \left(\frac{\partial m_{ij}}{\partial q_k} \right)_o \eta_k + \dots$$

Now T is already second order in the $\dot{\eta}$'s \rightarrow since we want lowest order, keep only first term in the m_{ij} . Let m_{ij} be elements of a square, real, symmetric matrix \mathbf{T} , and let the $\left(\frac{\partial V}{\partial q_i \partial q_j} \right)_o$ be the same for a matrix \mathbf{V} . How do we know \mathbf{V} is symmetric? It doesn't matter which order we take the partial derivatives in, so exchange of indices leaves the value unchanged.

So, we can express the Lagrangian as

$$\begin{aligned} L &= \frac{1}{2} \mathbf{T}_{ij} \dot{\eta}_i \dot{\eta}_j - \frac{1}{2} \mathbf{V}_{ij} \eta_i \eta_j \\ &= \frac{1}{2} \left(\frac{d\tilde{\boldsymbol{\eta}}}{dt} \cdot \mathbf{T} \cdot \frac{d\boldsymbol{\eta}}{dt} - \tilde{\boldsymbol{\eta}} \cdot \mathbf{V} \cdot \boldsymbol{\eta} \right) \end{aligned}$$

The equations of motion are:

$$T_{ij} \ddot{\eta}_j + V_{ij} \eta_j = 0$$

or in matrix notation:

$$\mathbf{T} \cdot \ddot{\boldsymbol{\eta}} + \mathbf{V} \cdot \boldsymbol{\eta} = 0 \quad \text{a linear ODE}$$

We have N equations, each may contain all the co-ordinates.

Note: T must be positive definite, because the kinetic energy must be positive:

$$\frac{d\tilde{\boldsymbol{\eta}}}{dt} \cdot \mathbf{T} \cdot \frac{d\boldsymbol{\eta}}{dt} > \mathbf{0}$$

In matrix language, T being positive definite (having positive eigenvalues) guarantees the kinetic energy will be positive no matter what $\boldsymbol{\eta}$ is (in other words, any matrix that obeys the above equation always is called positive definite).

As for our double pendulum example, we will seek solutions for which all the co-ordinates have the same oscillation frequency – the *normal modes*.

$$\boldsymbol{\eta} = \mathbf{a}_k e^{i\omega_k t}$$

where we should have as many normal modes as we have degrees of freedom. So, the EOM are

$$\begin{aligned} \mathbf{V} \cdot \boldsymbol{\eta} &= -\mathbf{T} \cdot \ddot{\boldsymbol{\eta}} = \omega^2 \mathbf{T} \cdot \boldsymbol{\eta} \\ V_{ij} a_j - \omega^2 T_{ij} a_j &= 0 \end{aligned}$$

and we have N linear homogeneous equations for the a 's. These have non-trivial solutions only if the determinant of the matrix formed by the coefficients vanishes:

$$\begin{vmatrix} V_{11} - \omega^2 T_{11} & V_{12} - \omega^2 T_{12} & \dots \\ V_{21} - \omega^2 T_{21} & V_{22} - \omega^2 T_{22} & \dots \\ \dots & \dots & \dots \end{vmatrix} = 0$$

We can write this as a modified eigenvalue equation. Let $\omega^2 = \lambda$

$$|\mathbf{V} - \lambda \mathbf{T}| = 0$$

which is a polynocial equation for λ . From the EOM, we get a characteristic (secular) equation for k^{th} eigenvector \mathbf{a}_k for the k^{th} normal mode (ie. for each root of λ – for each eigenvalue – substitute that root into the equations to get the ratio of the a_i 's, and these form the components of the eigenvector. We therefore have N eigenvalues/eigenvectors. Our modified eigenvalue equation is written

$$\mathbf{V} \cdot \mathbf{a}_k = \lambda_k \mathbf{T} \cdot \mathbf{a}_k$$

(called a modified eigenvalue eqn. since usually $\mathbf{V} \cdot \mathbf{a} = \lambda \mathbf{a}$).

We can show that the λ_k must be real. Take the transposed complex conjugate equation:

$$\mathbf{a}_l^\dagger \cdot \mathbf{V} = \lambda_l^* \mathbf{a}_l^\dagger \cdot \mathbf{T}$$

and dot it into \mathbf{a}_k

$$\mathbf{a}_l^\dagger \cdot \mathbf{V} \cdot \mathbf{a}_k - \lambda_l^* \mathbf{a}_l^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k = 0 = (\lambda_k - \lambda_l^*) \mathbf{a}_l^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k$$

and for $l = k$

$$(\lambda_k - \lambda_k^*) \mathbf{a}_k^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k = 0$$

let $\mathbf{a}_k = \boldsymbol{\alpha}_k + i\boldsymbol{\beta}_k$

$$\mathbf{a}_k^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k = \tilde{\boldsymbol{\alpha}}_k \cdot \mathbf{T} \cdot \boldsymbol{\alpha}_k + \tilde{\boldsymbol{\beta}}_k \cdot \mathbf{T} \cdot \boldsymbol{\beta}_k + i \left(\tilde{\boldsymbol{\alpha}}_k \cdot \mathbf{T} \cdot \boldsymbol{\beta}_k - \tilde{\boldsymbol{\beta}}_k \cdot \mathbf{T} \cdot \boldsymbol{\alpha}_k \right)$$

Now the last term vanishes because T is a symmetric matrix. So this proves $\mathbf{a}_k^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k$ is real (= twice the kinetic energy so additionally is >0). For $(\lambda_k - \lambda_k^*) \mathbf{a}_k^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k = 0$, we must have then $\lambda_k - \lambda_k^* = 0 \implies \lambda_k$ real.

Now

$$\lambda_k = \frac{\mathbf{a}_k^\dagger \cdot \mathbf{V} \cdot \mathbf{a}_k}{\mathbf{a}_k^\dagger \cdot \mathbf{T} \cdot \mathbf{a}_k}$$

The denominator is $2T > 0$, so if V is positive definite, the numerator is > 0 and λ_k are both real and positive, so we get stable oscillations and stable equilibria. Note however that if there exists an a_k such that

$$\mathbf{a}_k^\dagger \cdot \mathbf{V} \cdot \mathbf{a}_k < 0 \implies \lambda < 0, \omega^2 < 0$$

and ω is imaginary. The solution is then $a_k \propto e^{|\omega|t}$, and we have exponential growth. So this proves that V is a minimum for stable equilibrium. ie.

$$\mathbf{a}_k^\dagger \cdot \mathbf{V} \cdot \mathbf{a}_k = V > 0 \text{ for } \lambda > 0$$

In other words - we took our equilibrium to be at $V = 0$, so for stable equilibrium any other valid state must have larger potential energy.

Suppose that all the λ 's are distinct (ie. there are no degenerate roots)

$$(\lambda_k - \lambda_l^*) \tilde{\mathbf{a}}_k \cdot \mathbf{T} \cdot \mathbf{a}_l = 0$$

now $\lambda_k - \lambda_l^* \neq 0$ if $k \neq l$

$$\implies \tilde{\mathbf{a}}_k \cdot \mathbf{T} \cdot \mathbf{a}_l = 0 \text{ for } k \neq l$$

We therefore have an *orthogonality condition* for non-degenerate roots.

We can determine the ratio of elements of \mathbf{a}_k , but the normalization is undetermined. We usually normalize by requiring

$$\tilde{\mathbf{a}}_k \cdot \mathbf{T} \cdot \mathbf{a}_k = 1$$

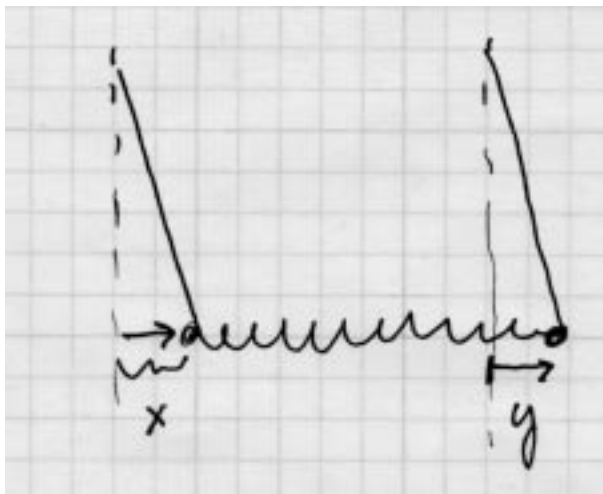
for each $\mathbf{a}_k \rightarrow$ we have N such equations. In general, let

$$\mathbf{A} = \begin{pmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_n \\ | & | & & | \\ | & | & & | \\ | & | & & | \end{pmatrix}$$

and we can write the normalization condition

$$\tilde{\mathbf{A}} \cdot \mathbf{T} \cdot \mathbf{A} = \bar{\mathbf{1}}$$

1.4 Example: Two coupled oscillators



Consider two coupled oscillators with the Lagrangian given by:

$$L = \frac{1}{2} (\dot{x}^2 + \dot{y}^2) - \frac{1}{2} \omega_o^2 (x^2 + y^2) + \alpha xy$$

where αxy is a coupling term. This type of Lagrangian could apply to two pendula of unit mass coupled by a spring, or electrical circuits coupled by mutual inductance. Note that if $\alpha = 0$, we have two independent oscillators with angular frequency ω_o .

The equations of motion are:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$$

We look for the normal mode solutions where $x, y \sim e^{i\omega t}$:

$$(\omega_o^2 - \omega^2) x - \alpha y = 0$$

$$(\omega_o^2 - \omega^2) y - \alpha x = 0$$

we get nontrivial solutions to these linear equations only if

$$\begin{vmatrix} \omega_o^2 - \omega^2 & \alpha \\ \alpha & \omega_o^2 - \omega^2 \end{vmatrix} = 0$$

so

$$\omega_o^2 - \omega^2 = \pm \alpha$$

$$\omega_{1,2}^2 = \omega_o^2 \mp \alpha$$

We find the ratios of the oscillation amplitudes for the eigenvectors by plugging the eigenfrequencies back into the linear equations:

$$\omega_1^2 = \omega_o^2 - \alpha \rightarrow A_x = A_y$$

$$\omega_2^2 = \omega_o^2 + \alpha \rightarrow A_x = -A_y$$

the eigenvectors are therefore:

$$\omega_1 = \sqrt{\omega_o^2 - \alpha} \quad \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

for the symmetric mode (where both pendula oscillate in the same direction), and

$$\omega_2 = \sqrt{\omega_o^2 + \alpha} \quad \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

for the antisymmetric mode, where they oscillate out of phase. This is a common characteristic – that the antisymmetric mode has higher frequency. If we call the eigenvector solutions θ_1, θ_2 then

$$x = \frac{\theta_1 + \theta_2}{\sqrt{2}}$$

$$y = \frac{\theta_1 - \theta_2}{\sqrt{2}}$$

For weak coupling, variations in x and y are the superposition of oscillations with nearly identical frequencies. We get a beat frequency phenomenon. To see this, look at the limit of weak coupling where $\alpha \ll \omega_o^2$,

$$\omega_1 \approx \omega_o \left(1 - \frac{1}{2} \frac{\alpha}{\omega_o^2} \right)$$

$$\omega_2 \approx \omega_o \left(1 + \frac{1}{2} \frac{\alpha}{\omega_o^2} \right)$$

so in this case

$$\begin{aligned} x &\propto e^{i\omega_o t \left(1 - \frac{1}{2} \frac{\alpha}{\omega_o^2}\right)} + e^{i\omega_o t \left(1 + \frac{1}{2} \frac{\alpha}{\omega_o^2}\right)} \\ &= \frac{1}{\sqrt{2}} e^{i\omega_o t} (e^{-i\omega_b t} + e^{i\omega_b t}) \end{aligned}$$

where we let $\omega_b = \frac{\alpha}{2\omega_o}$, so

$$x \propto e^{i\omega_o t} \cos \omega_b t$$

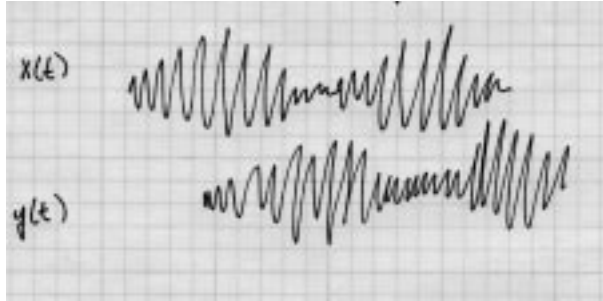
and

$$\begin{aligned} y &\propto e^{i\omega_o t \left(1 - \frac{1}{2} \frac{\alpha}{\omega_o^2}\right)} - e^{i\omega_o t \left(1 + \frac{1}{2} \frac{\alpha}{\omega_o^2}\right)} \\ &= \frac{1}{\sqrt{2}} e^{i\omega_o t} (e^{-i\omega_b t} - e^{i\omega_b t}) \end{aligned}$$

so

$$y \propto \frac{1}{\sqrt{2}} e^{i\omega_o t} \sin \omega_b t$$

So we can see that the beats are out of phase, and energy is exchanged between the two oscillators.



1.5 Normal Co-ordinates

We now illustrate the concept of normal co-ordinates, which are just the a_k 's. We can expand our generalized coordinates (the η 's) in terms of the eigenvectors (as we did above for x, y -

$$\eta(t) = C_k a_k e^{i\omega_k t}$$

where c_k is a complex amplitude factor, and a_k is a vector with real components. So the physical coordinates are a superposition of the normal modes. The complex amplitudes are then determined by the initial conditions, but the frequencies and phases of each mode, and the relative amplitudes of the motion of the η 's for that mode are characteristic of the mode.

A transformation into the normal coordinate system diagonalizes T and V , so that we can write for the k^{th} mode

$$\boldsymbol{\theta}_k = \text{Re} [c_k \mathbf{a}_k e^{i\omega t}]$$

(note here k isn't summed over), where $\boldsymbol{\theta}_k$ is the normal co-ordinate for that mode, and

$$L = \frac{1}{2} m_k \left(\dot{\boldsymbol{\theta}}_k^2 - \omega_k^2 \boldsymbol{\theta}_k^2 \right) \quad (\text{summed over } k)$$

in our previous example (ignoring the phase factor for now);

$$x \propto (\theta_1 + \theta_2)$$

$$y \propto (\theta_1 - \theta_2)$$

and

$$x \propto \text{Re} [(\cos \omega_o t + i \sin \omega_o t) \cos(\omega_b t)] \propto \cos \omega_o t \cos \omega_b t$$

$$y \propto \text{Re} [(\cos \omega_o t + i \sin \omega_o t)(-i \sin(\omega_b t))] \propto \sin \omega_o t \sin \omega_b t$$

so $x = x_{\text{max}}$ at $t = 0$, and $y = 0$ at $t = 0$. But, we can shift the phase (time) by multiplying by a complex constant.

1.6 Degeneracy

So far we have assumed that all roots of the secular equation are distinct. Nothing guarantees of course that the roots will be distinct, and we can have multiple $\lambda_l = \lambda_k$. We can then get two normal eigenvectors which will not, in general, be orthogonal. In this case we have to construct an orthogonal set. We can do this by taking a linear combination of the degenerate eigenvectors (which are linearly independent but not orthogonal).

Lets look at an example for the case of two degenerate roots corresponding to the normalized eigenvectors $\mathbf{a}_1, \mathbf{a}_2$ (remember we normalize them so that $\tilde{\mathbf{a}}_1 \cdot \mathbf{T} \cdot \mathbf{a}_1 = 1$). We construct a third vector

$$\mathbf{a}_3 = c_1 \mathbf{a}_1 + c_2 \mathbf{a}_2$$

We want to make $\tilde{\mathbf{a}}_1 \cdot \mathbf{T} \cdot \mathbf{a}_3 = 0$.

$$\tilde{\mathbf{a}}_3 \cdot \mathbf{T} \cdot \mathbf{a}_1 = c_1 + c_2 (\tilde{\mathbf{a}}_2 \cdot \mathbf{T} \cdot \mathbf{a}_1) = 0$$

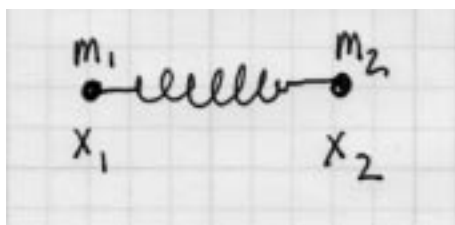
$$\frac{c_1}{c_2} = -\tilde{\mathbf{a}}_2 \cdot \mathbf{T} \cdot \mathbf{a}_1$$

also,

$$\tilde{\mathbf{a}}_3 \cdot \mathbf{T} \cdot \mathbf{a}_3 = 1 = c_1^2 + c_2^2 + 2c_1 c_2 (\tilde{\mathbf{a}}_2 \cdot \mathbf{T} \cdot \mathbf{a}_1) = 1$$

(Note: $\tilde{\mathbf{a}}_1 \cdot \mathbf{T} \cdot \mathbf{a}_2 = \tilde{\mathbf{a}}_2 \cdot \mathbf{T} \cdot \mathbf{a}_1$ since T is symmetric). We have two independent equations that we can solve for c_1 and c_2 . We then use \mathbf{a}_3 and \mathbf{a}_1 as our orthogonal eigenvectors. They are automatically orthogonal to the other (non-degenerate) vectors. This is called the Gram-Schmidt process. We can follow the same procedure for higher multiplicity roots also.

Note that even though the λ 's are degenerate, the modes describe different motions of the system (which happen to have the same frequency).



1.7 Molecular Vibrations

Consider a diatomic molecule – a physical system that can be approximated by two masses coupled by a spring:

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 - \frac{1}{2}k(x_1 - x_2)^2$$

The Euler-Lagrange equations give us

$$m_1\ddot{x}_1 + k(x_1 - x_2) = 0$$

$$m_2\ddot{x}_2 + k(x_2 - x_1) = 0$$

and we get the eigenfrequencies from

$$\begin{vmatrix} m_1\omega^2 - k & k \\ k & m_2\omega^2 - k \end{vmatrix} = 0$$

$$(m_1\omega^2 - k)(m_2\omega^2 - k) - k^2 = 0$$

the roots are

$$\omega^2 = 0, \frac{k}{\mu}$$

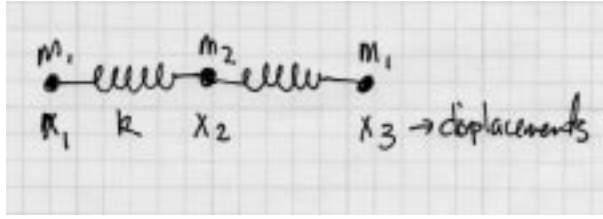
where $\mu = \frac{m_1 m_2}{m_1 + m_2}$. What does the root $\omega = 0$ correspond to? It is associated with a non-oscillatory motion of the system, ie. translation of the center of mass. $\omega^2 = k/\mu$ corresponds to vibration about the center of mass. Our normal coordinates are for $\omega = 0, x_1 = x_2$. $x_1 = x_2$ clearly corresponds to a translation of the system. We can remove this by considering only motion about the CM, thereby reducing the number of degrees of freedom. This will help with larger numbers of atoms.

1.7.1 The linear, symmetric, triatomic molecule

As seen in the previous example, we would like to first suppress the center of mass motion. To do this, we make the total momentum = 0. The CM at rest implies

$$m_1x_1 + m_2x_2 + m_3x_3 = 0$$

$$x_2 = -\frac{m_1}{m_2}(x_1 + x_3)$$



We can use this to eliminate one or our coordinates, reducing the dimension of the problem by one

$$L = \frac{1}{2}m_1 (\dot{x}_1^2 + \dot{x}_3^2) + \frac{1}{2}m_2\dot{x}_2^2 - \frac{1}{2}k [(x_1 - x_2)^2 + (x_2 - x_3)^2]$$

eliminate x_2 , and do a lot of algebra, and we find

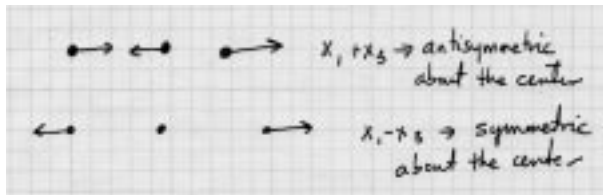
$$L = \frac{m_1 M}{2m_2} \dot{Q}_a^2 + \frac{m_1}{2} \dot{Q}_s^2 - \frac{k M^2}{2m_2^2} Q_a^2 - \frac{k}{2} Q_s^2$$

where

$$Q_a = \frac{x_1 + x_3}{\sqrt{2}}$$

$$Q_s = \frac{x_1 - x_3}{\sqrt{2}}$$

and $M = 2m_1 + m_2$ is the total mass. These motions correspond to our normal modes – which we could have guessed physically:



Our "masses/spring constant" are m_1/k and $\frac{m_1 M}{m_2} / \frac{k M^2}{m_2^2}$ so the normal frequencies $\omega' = \sqrt{\frac{k'}{m'}}$ are

$$\omega_1^2(\text{symmetric}) = \frac{k}{m_1}$$

$$\omega_2^2(\text{antisymmetric}) = \frac{k M}{m_1 m_2}$$

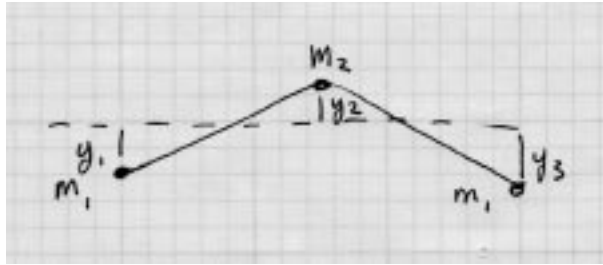
There is also a transverse mode of oscillation.

Again, we reduce the degrees of freedom by removing the CM motion, but in this case also rotation:

$$m_1 (y_1 + y_3) = m_2 y_2 \quad - \text{suppress translation}$$

Now we also want to suppress rotation in the plane of the molecule, so use conservation of angular momentum

$$\mathbf{r}_a = \mathbf{r}_{a0} + \mathbf{u}_a$$



where \mathbf{u}_a is the displacement from equilibrium, and the angular momentum

$$\begin{aligned} \mathbf{L} &= \sum_a m_a \mathbf{r}_a \times \mathbf{v}_a \approx \sum_a m_a \mathbf{r}_{a0} \times \dot{\mathbf{u}}_a \\ &= \frac{d}{dt} \left(\sum_a m_a \mathbf{r}_{a0} \times \mathbf{u}_a \right) = 0 \end{aligned}$$

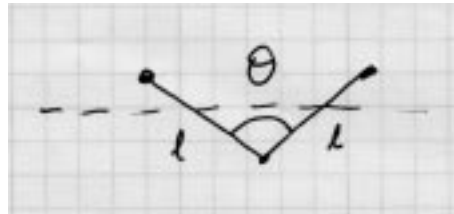
and since we can choose the origin arbitrarily,

$$\sum_a m_a \mathbf{r}_{a0} \times \mathbf{u}_a = 0$$

For our molecule, this implies:

$$y_1 = y_3 \quad (\text{supress rotation})$$

Now we write the Lagrangian. Let δ be the deviation of θ from π .



$$\delta = \left[\frac{y_1 - y_2}{l} + \frac{y_3 - y_2}{l} \right]$$

The potential energy

$$V = \frac{1}{2} k' l^2 \delta^2$$

and $k_2 = k' l^2$

$$L = \frac{1}{2} m_1 (\dot{y}_1^2 + \dot{y}_3^2) + \frac{1}{2} m_2 \dot{y}_2^2 - \frac{1}{2} k' (y_1 + y_3 + 2y_2)^2$$

We use our two constraints ($y_1 = y_3$, $2y_1 \frac{m_1}{m_2} = y_2$) to remove y_2 and y_3 :

$$L = m_1 \dot{y}_1^2 + \frac{2m_1^2}{m_2} \dot{y}_1^2 - \frac{4}{2} k' \left(y_1 + \frac{2m_1}{m_2} y_1 \right)^2$$

From the E-L equations:

$$2 \left(m_1 + 2 \frac{m_1^2}{m_2} \right) \ddot{y}_1 = -4k' \left(1 + \frac{2m_1}{m_2} \right)^2 y_1$$

so

$$\omega^2 = 2k' \frac{M}{m_1 m_2}$$

In general, if we have N atoms, we have $3N$ degrees of freedom. $3N-6$ correspond to vibration (we subtract 6 – 3 for translation and 3 for rotation). For co-linear atoms, we have $3N-5$ dof, since rotation about the line of the atoms is not significant. For a linear molecule, $n-1$ are in line, so $2n-4$ bring the atom out of line. Here both have the same frequency (2 mutually perpendicular planes).