Chapter 3

Vibrations & Oscillations

The topic of vibrations and oscillations is typically discussed in some detail in a course on waves (at MIT this is 8.03). Our goal for this chapter is to revisit aspects of oscillation phenomena using generalized coordinates. Many equations of motion we have encountered have been nonlinear. Here, we will expand about a minimum of the potential $V(q_1, \ldots, q_n)$, yielding linear equations.

Let us take $q_i = q_{0i} + \eta_i$, where $\vec{q}_0$ minimizes $V(q)$, and expand in the η_i. Henceforth and until further notice, repeated indices will implicitly be summed over. Then

$$V(q_1, \ldots, q_n) = V(q_{01}, \ldots, q_{0n}) + \left.\frac{\partial V}{\partial q_i}\right|_0 \eta_i + \frac{1}{2}\left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_0 \eta_i \eta_j + \ldots, \tag{3.1}$$

where $|_0$ means "evaluate the quantity at $\vec{q}_0$". We already know that $\left.\frac{\partial V}{\partial q_i}\right|_0 = 0$ as by definition $\vec{q}_0$ minimizes $V(q)$. As a matter of convention, we choose $V(q_0) = 0$, since this just corresponds to picking the convention for the zero of the Energy. Finally, we define the constants $V_{ij} \equiv \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_0$. There is no time dependence in the definition of our generalized coordinates, so the kinetic energy is

$$T = \frac{1}{2} m_{ij}(q_1, \ldots, q_n)\dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij}(q_{01}, \ldots, q_{0n})\dot{\eta}_i \dot{\eta}_j + \mathcal{O}(\eta\dot{\eta}^2), \tag{3.2}$$

where $m_{ij}(q_{01}, \ldots, q_{0n}) \equiv T_{ij}$ are constants, and terms of $\mathcal{O}(\eta\dot{\eta}^2)$ and beyond are neglected. Thus, the Lagrangian to quadratic order in the η_is is

$$L = \frac{1}{2}\left(T_{ij}\dot{\eta}_i \dot{\eta}_j - V_{ij}\eta_i \eta_j\right). \tag{3.3}$$

From this, the equations of motion are

$$T_{ij}\ddot{\eta}_j + V_{ij}\eta_j = 0 \tag{3.4}$$

to the same order. These are coupled linear equations of motion.

3.1 Simultaneous Diagonalization of $\hat{T}$ and $\hat{V}$

To solve Eq. (3.4) lets try

$$\eta_i = a_i e^{-\mathrm{i}\omega t} \tag{3.5}$$

where $a_i \in \mathbb{C}$ for all $i \in \{1, \ldots, n\}$, and the frequency ω is the same along all directions in the generalized coordinate space. Notationally, i and j will denote coordinate indices, while $\mathrm{i} = +\sqrt{-1}$ is the imaginary unit. This gives

$$V_{ij} a_j = \omega^2 T_{ij} a_j \tag{3.6}$$

which can be rewritten in matrix form as

$$\hat{V} \cdot \vec{a} = \lambda \hat{T} \cdot \vec{a} \tag{3.7}$$

with $\lambda = \omega^2$. This looks like an eigenvalue equation except that when we act with the linear operator $\hat{V}$ on $\vec{a}$ we get back $\hat{T} \cdot \vec{a}$ instead of just the eigenvector $\vec{a}$. This can be rewritten as

$$(\hat{V} - \lambda \hat{T}) \cdot \vec{a} = 0 \tag{3.8}$$

where $\hat{V}$ and $\hat{T}$ are *real* and *symmetric* $n \times n$ matrices. In order to have a non-trivial solution of this equation we need

$$\det(\hat{V} - \lambda \hat{T}) = 0 \tag{3.9}$$

which is an n^{th} order polynomial equation with n solutions eigenvalues λ_α with $\alpha \in \{1, \ldots, n\}$. The solutions of $(\hat{V} - \lambda_\alpha \hat{T}) \cdot \vec{a}^{(\alpha)} = 0$ are the eigenvectors $\vec{a}^{(\alpha)}$. This means

$$\hat{V} \cdot \vec{a}^{(\alpha)} = \lambda_\alpha \hat{T} \cdot \vec{a}^{(\alpha)} \,, \tag{3.10}$$

and the solutions are much like a standard eigenvalue problem. Here and henceforth, there will be no implicit sum over repeated eigenvalue indices α (so any sums that are needed will be made explicit), but we will retain implicit sums over repeated coordinate indices i & j.

There are two cases we will consider.

1) Let us start by considering the case when $\hat{T}$ is diagonal. In particular, let us consider the even easier case proportional to the unit matrix, where $T_{ij} = m\delta_{ij}$. This means

$$m\ddot{\eta}_i + V_{ij}\eta_j = 0 \,. \tag{3.11}$$

Here we have the standard eigenvalue equation

$$\hat{V} \cdot \vec{a}^{(\alpha)} = m\lambda_\alpha \vec{a}^{(\alpha)} \,. \tag{3.12}$$

The eigenvalues λ_α are real and nonnegative as $\lambda_\alpha = \omega_\alpha^2$; the quantities ω_α are the *normal mode frequencies*. The eigenvectors $\vec{a}^{(\alpha)}$ are orthogonal, and we can choose their normalization so that

$$m\,\vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)} = \delta_{\beta\alpha} \qquad (\text{or } \vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)} = \delta_{\beta\alpha})\,. \tag{3.13}$$

This implies that

$$\lambda_\alpha = \vec{a}^{(\alpha)\dagger}\cdot\hat{V}\cdot\vec{a}^{(\alpha)} \qquad (\text{or } m\lambda_\alpha = \vec{a}^{(\alpha)\dagger}\cdot\hat{V}\cdot\vec{a}^{(\alpha)})\,. \tag{3.14}$$

The time-dependent eigenvectors are then

$$\vec{\eta}^{(\alpha)} = \vec{a}^{(\alpha)}e^{-\mathrm{i}\omega_\alpha t}, \quad \text{or} \quad \eta_i^{(\alpha)} = a_i^{(\alpha)}e^{-i\omega_\alpha t}. \tag{3.15}$$

These are the normal mode solutions for the n coordinates labeled by i, and there are n such solutions labeled by α. The general solution of a linear equation is a superposition of the independent normal mode solutions:

$$\vec{\eta} = \sum_\alpha C_\alpha\,\vec{\eta}^{(\alpha)} \tag{3.16}$$

where $C_\alpha \in \mathbb{C}$ are fixed by initial conditions. To find real coordinate solutions, we take the real parts of these equations.

Lets prove the statements made above. Again, there will be no implicit sum over the eigenvalue index α. Dotting in $\vec{a}^{(\beta)\dagger}$ into Eq. (3.12) gives

$$\vec{a}^{(\beta)\dagger}\cdot\hat{V}\cdot\vec{a}^{(\alpha)} = m\lambda_\alpha\vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)}\,, \tag{3.17}$$

taking the Hermitian conjugate of both sides, noting that $\hat{V}^\dagger = \hat{V}$, and then swapping $\alpha \leftrightarrow \beta$ gives $\vec{a}^{(\beta)\dagger}\cdot\hat{V}\cdot\vec{a}^{(\alpha)} = m\lambda_\beta^\star\vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)}$. Taking the difference of these results gives

$$(\lambda_\alpha - \lambda_\beta^\star)\vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)} = 0, \tag{3.18}$$

and if $\alpha = \beta$ then $(\lambda_\alpha - \lambda_\alpha^\star)\vec{a}^{(\alpha)\dagger}\cdot\vec{a}^{(\alpha)} = 0$ implies the eigenvalues are real $\lambda_\alpha \in \mathbb{R}$. For $\lambda_\alpha \neq \lambda_\beta$, Eq. (3.18) then implies $\vec{a}^{(\beta)\dagger}\cdot\vec{a}^{(\alpha)} = 0$ so the eigenvectors are orthogonal. If by chance $\lambda_\alpha = \lambda_\beta$ for some $\alpha \neq \beta$ then we can always simply choose the corresponding eigenvectors to be orthogonal. By convention, we then normalize the eigenvectors so that they satisfy Eq. (3.13). Finally, if $\alpha = \beta$ then Eq. (3.17) now gives $\lambda_\alpha = \vec{a}^{(\alpha)\dagger}\cdot\hat{V}\cdot\vec{a}^{(\alpha)}$. The statement that we are at a local minimum of the multivariable potential and not a saddle point or a maximum implies then that $\lambda_\alpha \geq 0$ (we have positive second derivatives in each eigenvector direction).

2) Let us now consider when $\hat{T}$ is not diagonal and summarize which parts of the result are the same and where there are differences. Here we have $(\hat{V} - \lambda\hat{T})\cdot\vec{a} = 0$. Again, the eigenvalues λ_α are real and nonnegative, with $\lambda_\alpha = \omega_\alpha^2$. Now, however,

$$\vec{a}^{(\beta)\dagger}\cdot\hat{T}\cdot\vec{a}^{(\alpha)} = 0\,, \tag{3.19}$$

for $\alpha \neq \beta$, and we can replace the old normalization condition by a new one stating that

$$\vec{a}^{(\beta)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)} = \delta_{\alpha\beta}, \tag{3.20}$$

which up to an overall prefactor reduces to the old orthonormality condition when $\hat{T} = m\hat{1}$. Here again,

$$\lambda_\alpha = \vec{a}^{(\alpha)\dagger} \cdot \hat{V} \cdot \vec{a}^{(\alpha)}\,, \tag{3.21}$$

and the α^{th} normal mode solution is

$$\vec{\eta}^{(\alpha)} = \vec{a}^{(\alpha)} e^{-\mathrm{i}\omega_\alpha t}\,. \tag{3.22}$$

The general solution is again the superposition

$$\vec{\eta} = \sum_\alpha C_\alpha \vec{\eta}^{(\alpha)}\,, \tag{3.23}$$

with the complex coefficients C_α fixed by the initial conditions (and a real part taken to get real coordinates).

Lets repeat the steps of our proof for this case. Dotting $\vec{a}^{(\beta)\dagger}$ into Eq. (3.10) gives

$$\vec{a}^{(\beta)\dagger} \cdot \hat{V} \cdot \vec{a}^{(\alpha)} = \lambda_\alpha \vec{a}^{(\beta)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)}\,. \tag{3.24}$$

Taking the Hermitian conjugate of both sides yields $\vec{a}^{(\beta)\dagger} \cdot \hat{V} \cdot \vec{a}^{(\alpha)} = \lambda_\beta^\star \vec{a}^{(\beta)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)}$. Subtracting the two results this gives

$$(\lambda_\alpha - \lambda_\beta^\star)\, \vec{a}^{(\beta)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)} = 0, \tag{3.25}$$

and if $\alpha = \beta$ then $(\lambda_\alpha - \lambda_\alpha^\star)\vec{a}^{(\alpha)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)} = 0$ implies $\lambda_\alpha \in \mathbb{R}$ since $\hat{T} = \hat{T}^\star = \hat{T}^\top$ and physically we know that the kinetic energy $T = \dot{\vec{\eta}} \cdot \hat{T} \cdot \dot{\vec{\eta}} > 0$ for any $\dot{\vec{\eta}} \neq 0$. For $\lambda_\alpha \neq \lambda_\beta$, then the condition instead implies $\vec{a}^{(\beta)\dagger} \cdot \hat{T} \cdot \vec{a}^{(\alpha)} = 0$ so the eigenvectors are orthogonal; if by chance $\lambda_\alpha = \lambda_\beta$ for some $\alpha \neq \beta$ then we can choose the corresponding eigenvectors to be orthogonal. By convention, we normalize the eigenvectors so that they will be orthonormal as in Eq. (3.20). Finally, if $\alpha = \beta$ then $\lambda_\alpha = \vec{a}^{(\alpha)\dagger} \cdot \hat{V} \cdot \vec{a}^{(\alpha)}$, which is positive, so $\lambda_\alpha > 0$ also. The statement that we are at a local minimum of the potential and not a saddle point or a maximum implies then that $\lambda_\alpha \geq 0$.

3.2 Vibrations and Oscillations with Normal Coordinates

Given these results, it is natural to ask whether a different set of generalized coordinates might be better for studying motion about the minimum?

We form the matrix A by placing the eigenvectors in columns

$$A = \begin{bmatrix} \vec{a}^{(1)} & \vec{a}^{(2)} & \dots & \vec{a}^{(n)} \end{bmatrix} \tag{3.26}$$

and construct a diagonal eigenvalue matrix $\hat{\lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. The matrix A can be ensured to be real because each $\vec{a}^{(\alpha)}$ only has at most an overall phase[1], and these can be removed by putting them into the coefficients C_α. The matrix A simultaneously diagonalizes $\hat{T}$ and $\hat{V}$ since

$$A^\top \hat{T} A = \mathbb{1} \quad \text{and} \quad A^\top \hat{V} A = \hat{\lambda}. \tag{3.27}$$

We choose new *normal coordinates* $\vec{\xi}$ by letting

$$\vec{\eta} = A\,\vec{\xi} \quad \text{and} \quad \dot{\vec{\eta}} = A\,\dot{\vec{\xi}} \tag{3.28}$$

so that the Lagrangian

$$\begin{aligned} L &= \frac{1}{2}\dot{\vec{\eta}} \cdot \hat{T} \cdot \dot{\vec{\eta}} - \frac{1}{2}\vec{\eta} \cdot \hat{V} \cdot \vec{\eta} \\ &= \frac{1}{2}\dot{\vec{\xi}} \cdot (A^\top \hat{T} A) \cdot \dot{\vec{\xi}} - \frac{1}{2}\vec{\xi} \cdot (A^\top \hat{V} A) \cdot \vec{\xi} \\ &= \frac{1}{2}\sum_\alpha \left(\dot{\xi}_\alpha^2 - \omega_\alpha^2 \xi_\alpha^2 \right) . \end{aligned} \tag{3.29}$$

This gives the simple equations of motion for each α:

$$\ddot{\xi}_\alpha + \omega_\alpha^2\, \xi_\alpha = 0\,. \tag{3.30}$$

Thus, each normal coordinate describes the oscillations of the system with normal mode frequency ω_α.

Example: Let us consider the triatomic molecule CO_2 shown in Figure 3.1. We can picture it as a carbon atom of mass M in the middle of two oxygen atoms each of mass m. For the three particles there are 9 coordinates given by $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$. Six of these coordinates correspond to translations and rotations of the mass system treated as a rigid body. This leaves 3 coordinates that correspond to internal motions of the system. To model the potential we connect each oxygen atom to the carbon atom with a spring of constant k and relaxed length b. This does not add any cost to relative motion of the atoms with fixed spring length, which we will address below by adding another potential term in order to favor the linear configuration.

It is straightforward to guess what the normal modes could be:

[1] Why is it just an overall phase? The equation $\hat{V} \cdot \vec{a}^{(\alpha)} = \lambda_\alpha \hat{T} \cdot \vec{a}^{(\alpha)}$ alone does not fix the normalization of $\vec{a}^{(\alpha)}$. Let us say we pick $a_i^{(\alpha)} \in \mathbb{R}$ for some i. Then $V_{kj} a_j^{(\alpha)} = \lambda_\alpha K_{kj} a_j^{(\alpha)}$ is a set of equations with all real coefficients and one real term in the sums. Hence the solutions $a_j^{(\alpha)}/a_i^{(\alpha)} \in \mathbb{R}$ for all $j \in \{1, \dots, n\}$, implying that at most there is an overall phase in $\vec{a}^{(\alpha)}$.

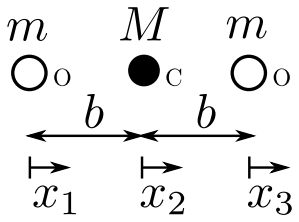

Figure 3.1: The CO_2 molecule.

- The oxygen atoms moving in the same direction along the line and the carbon atom moving in the opposite direction. This is a longitudinal oscillation.
- The oxygen atoms opposing each other along the line while the carbon atom remains at rest. This is a longitudinal oscillation.
- The oxygen atoms move in the same direction perpendicular to the line and the carbon atom moving in the opposite direction. This is a transverse oscillation.

These three normal modes are shown in Figure 3.2.

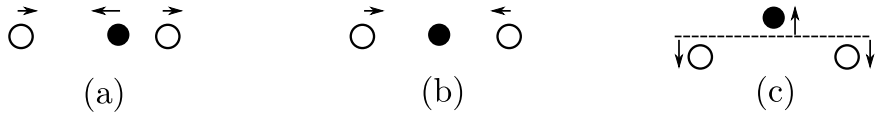

Figure 3.2: The three Normal Modes of the CO_2 molecule

We pick the body frame axes as follows:

- the three particles are in the xy-plane fixing 3 coordinates $z_i = 0$ for $i \in \{1, 2, 3\}$,
- the origin is the CM so $m(x_1 + x_3) + Mx_2 = m(y_1 + y_3) + My_2 = 0$, which fixes two more coordinates,
- the axes are oriented so that $y_1 = y_3$, which fixes one coordinate.

Defining the mass ratio as $\rho \equiv \frac{m}{M}$, then $x_2 = -\rho(x_1 + x_3)$ and $y_2 = -2\rho y_1$ can be eliminated. Altogether this fixes 6 coordinates, leaving the coordinates (x_1, x_3, y_1). This setup is shown in Figure 3.3.

For the potential we take

$$V = \frac{k}{2}(s_1 - b)^2 + \frac{k}{2}(s_2 - b)^2 + \frac{\lambda b^2}{2}(\alpha_1^2 + \alpha_2^2)\,. \tag{3.31}$$

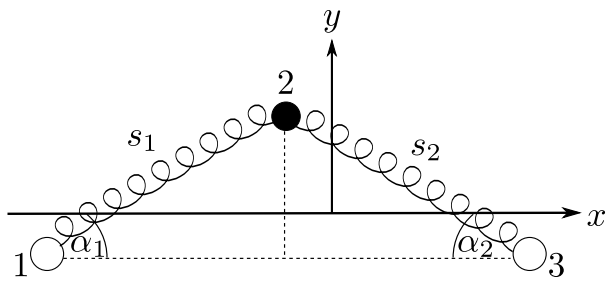

Figure 3.3: The orientation of the CO_2 molecule on xy plane

The first two terms are the springs discussed previously, and the last two provide a quadratic energy cost to the springs rotating away from the linear configuration, with strength given by λ. The spring lengths are

$$s_1 = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} = \sqrt{[x_1 + \rho(x_1 + x_3)]^2 + (1 + 2\rho)^2 y_1^2} \tag{3.32}$$
$$s_2 = \sqrt{(x_2 - x_3)^2 + (y_2 - y_3)^2} = \sqrt{[x_3 + \rho(x_1 + x_3)]^2 + (1 + 2\rho)^2 y_1^2}\,,$$

and the two angles are

$$\alpha_1 = \tan^{-1}\left(\frac{y_3 - y_2}{x_3 - x_2}\right) = \tan^{-1}\left[\frac{(1 + 2\rho)y_1}{(1 + \rho)x_1 + x_3}\right], \tag{3.33}$$
$$\alpha_2 = \tan^{-1}\left(\frac{y_2 - y_1}{x_2 - x_1}\right) = \tan^{-1}\left[\frac{(1 + 2\rho)y_1}{(1 + \rho)x_3 + x_1}\right].$$

These results give $V = V(x_1, x_3, y_1)$. [to be continued]

For the kinetic energy we have

$$T = \frac{m}{2}\left(\dot{x}_1^2 + \dot{x}_3^2\right) + \frac{M}{2}\dot{x}_2^2 + \frac{m}{2}\left(\dot{y}_1^2 + \dot{y}_3^2\right) + \frac{M}{2}\dot{y}_2^2, \tag{3.34}$$

which after eliminating coordinates becomes

$$T = \frac{m}{2}\left(1+\rho\right)\left(\dot{x}_1^2 + \dot{x}_3^2\right) + m\rho\dot{x}_1\dot{x}_3 + m\left(1+2\rho\right)\dot{y}_1^2. \tag{3.35}$$

Equilibrium comes from taking $y_1 = 0$, $x_3 = -x_1 = b$, which implies $\alpha_1 = \alpha_2 = 0$, $s_1 = s_2 = b$, and $V = 0$. We define coordinates for expanding about this potential minimum as $\eta_1 = x_1 + b$, $\eta_3 = x_3 - b$, and $\eta_2 = y_1$. Then as $V(-b, b, 0) = 0$ in equilibrium and $\frac{\partial V}{\partial \eta_i}\Big|_0 = 0$ then $V = \frac{1}{2}V_{ij}\eta_i\eta_j + \ldots$ where

$$V_{ij} = \left.\frac{\partial^2 V}{\partial\eta_i\partial\eta_j}\right|_0 = \begin{bmatrix} k(1+2\rho+2\rho^2) & 0 & 2k\rho(1+\rho) \\ 0 & 2\lambda(1+2\rho)^2 & 0 \\ 2k\rho(1+\rho) & 0 & k(1+2\rho+2\rho^2) \end{bmatrix} \tag{3.36}$$

for this system. Additionally,

$$T_{ij} = \begin{bmatrix} m(1+\rho) & 0 & m\rho \\ 0 & 2m(1+2\rho) & 0 \\ m\rho & 0 & m(1+\rho) \end{bmatrix} \tag{3.37}$$

for this system. Since there are no off-diagonal terms in the 2nd row or 2nd column in either $\hat{V}$ or $\hat{T}$, the transverse and the longitudinal modes decouple. For the transverse mode, we are left with

$$\ddot{y}_1 + \frac{2\lambda(1+2\rho)^2}{2m(1+2\rho)}y_1 = 0\,, \tag{3.38}$$

which is a simple harmonic oscillator. For the longitudinal modes, we have $\vec{\eta} = (\eta_1, \eta_3)$. The frequencies come from

$$\det\begin{bmatrix} k(1+2\rho+2\rho^2) - \lambda m(1+\rho) & 2k\rho(1+\rho) - \lambda m\rho \\ 2k\rho(1+\rho) - \lambda m\rho & k(1+2\rho+2\rho^2) - \lambda m(1+\rho) \end{bmatrix} = 0 \tag{3.39}$$

The solutions give the normal mode frequencies

$$\lambda_1 = \omega_1^2 = \frac{k}{m}\,, \qquad \lambda_2 = \omega_2^2 = \frac{k}{m}\left(1+2\rho\right)\,, \tag{3.40}$$

with associated eigenvectors

$$\vec{a}^{(1)} = \frac{1}{\sqrt{2m}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\,, \qquad \vec{a}^{(2)} = \frac{1}{\sqrt{2m(1+2\rho)}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\,, \tag{3.41}$$

which were chosen to satisfy $\vec{a}^{(\alpha)} \cdot \hat{T} \cdot \vec{a}^{(\beta)} = \delta_{\alpha\beta}$. Thus, the normal coordinates for the longitudinal modes are $\xi_1 \propto x_1 - x_3$ and $\xi_2 \propto x_1 + x_3$. Oscillations in these coordinates correspond to the normal mode motions in Fig. 3.2(b) and Fig. 3.2(a) respectively.

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8.09 Classical Mechanics III

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