Oscillations

Consider the minimum of a potential $V(\vec{q}_0)$ around the point of minimum $(q_0_1, q_0_2, \ldots, q_0_n) \equiv \vec{q}_0$

We may expand in a Taylor series as

$$V(\vec{q}; \vec{q}_0) = V(q_0_1, q_0_2 + \ldots, q_0_n) + \sum_i \frac{\partial V}{\partial q_i}(\vec{q} - \vec{q}_0)_i^2 + \ldots$$

Note $\vec{q} = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix}$

At the minimum $\frac{\partial V}{\partial q_i} = 0$, for all $i$

Also, if we subtract the constant term $V(q_0_1, q_0_2, \ldots, q_0_n)$ from the definition of $V$ we get

$$V(\vec{q}; \vec{q}_0) = \sum_i \frac{\partial^2 V}{\partial q_i^2} (\vec{q} - \vec{q}_0)_i^2 (q_i - q_{0i})(q_j - q_{0j})$$
neglecting higher order terms for small deviations \( |\vec{q} - \vec{q}_0| \).

The kinetic energy may be written as

\[ T = \sum \frac{m_i}{2} \dot{q}_i \dot{q}_i \]

when we have no explicit time dependence in the generalized coordinates as seen from Eq \( (6.71) \).

\( m_i \) are in general \( m_i = m_i(\vec{q}_i) \).

But to lowest order in the \( \vec{q}_i \)'s we get

\[ m_i(\vec{q}) = m_i(\vec{q}_0) = \text{constant} \]

Let then \( T = T(\vec{q}_0) \)

\[ \Rightarrow T = \frac{1}{2} \ddot{\vec{q}}^T \ddot{\vec{q}} = \frac{1}{2} \sum \ddot{q}_i \ddot{q}_i \]

\[ L = T - V = \frac{1}{2} \left[ \ddot{\vec{q}}^T \ddot{\vec{q}} - \vec{q}^T \nabla \vec{q} \right] \] \( \Rightarrow (6.7) \)

\[ \Rightarrow \frac{\partial L}{\partial \dot{\vec{q}}} - \ddot{\vec{q}} = 0 \]

\[ \Rightarrow \ddot{\vec{q}} + \nabla \vec{q} = 0 \] \( \Rightarrow (6.8) \)
In writing $\nabla^T \nabla \bar{q} = 2V$ we implicitly assumed $\bar{q}_0 = 0$. This is trivially done by saying $\bar{q}_n = \bar{q} - \bar{q}_0$.

$$\bar{q}_n = \bar{q} \quad \Rightarrow \quad V = \bar{q}_n^T \nabla \bar{q}_n$$

$$T = \bar{q}_n^T \nabla \bar{q}_n$$

Now rename $\bar{q}_n$ back as $\bar{q}$.

Eq. 6.3 gives

$$\bar{q}_n^T \nabla \bar{q} = -\nabla \bar{q}$$

$$\nabla \bar{q} = -\bar{q}^T \nabla \bar{q}$$

Let $\{\lambda_k\}$ be the non-degenerate eigenvalues and $\{\bar{a}_k\}$ be the eigenvectors of $\bar{q} = \bar{q}^T \nabla \bar{q}$.

Note non-degenerate $\Rightarrow \lambda_k \neq \lambda_j, \forall j$. 

$$\therefore \quad \bar{q} = \bar{q}^T \nabla \bar{a}_k = \lambda_k \bar{a}_k$$

$$\bar{a}_k \equiv \begin{bmatrix} a_{k1} \\ a_{k2} \\ \vdots \\ a_{kn} \end{bmatrix}_{n \times 1}$$
Let \( \hat{e}_k \) be unit vectors \( \exists \)

\[
e_{k:k} = \delta_{x:k}
\]

i.e., \( \hat{e}_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \), a column with all zeros but 1 at the \( k \) th row.

Define

\[
\overline{A} = \sum_{k} \hat{e}_k \cdot \overline{a}_k^T
\]

\( \Rightarrow \) \( A_{ij} = \left[ \sum_k \hat{e}_k \cdot \overline{a}_k^T \right]_{ij} \)

\[
= \sum_k e_{ki} a_{kj} = \sum_k s_{ik} a_{kj} = a_{ij}
\]

\( \Rightarrow \) The \( k \) th column of \( \overline{A} \) is \( \overline{a}_k \).

\[
\therefore \quad \overline{A}^{-1} \overline{a}_k = \lambda_k \overline{a}_k \]

\( \Rightarrow \) \( \overline{a}_k = \lambda_k \overline{A}^{-1} \overline{a}_k \)

\( \Rightarrow \) \( \overline{\overline{A}} = \overline{\lambda} \overline{A} \)

where \( \overline{A} \) is a \( nxn \) matrix which is diagonal \( \Rightarrow \) \( a_{ij} = \delta_{ij} \delta_{ij} \)

Define the Hermitian conjugate by a dagger superscript \( ^\dagger \)
\[ B^+ = (B^*)^* = (B^*)^T \]

where \( B^* \) is conjugate transpose of \( B \), i.e., where \( (B^*)_{ij} = (B_{ij})^* = B^*_{ij} \)

where * denotes complex conjugation.

\((a + ib)^* = a - ib\) or \((re^{iθ})^* = re^{-iθ}\) where \( r \) is a real number.

\( \overline{\overline{\nu}} \) and \( \overline{T} \) are real and also

\( \overline{\overline{\nu}}^T = \overline{\nu} \) & \( \overline{T}^T = \overline{T} \)

\[ \overline{\overline{\nu}^T} = \overline{\nu} \] & \( \overline{T}^T = \overline{T} \)

Eq. (6.155) gives \( \overline{\overline{A}} = A^T\overline{A} \)

\[ A^T\overline{A} = A^T\overline{A} \]

\[ (A^T\overline{A})^* = (A^T\overline{A})^T \]

\[ \overline{A^T\overline{A}} = \overline{A^T\overline{A}} \]

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\[ A^T = \overline{A}^* \]

\( A \) is diagonal \( \Rightarrow \overline{A^T} = \overline{A}^* \)

\( \overline{A^T} = \overline{A}^T \Rightarrow A = A^+ \)

\( \overline{A} \) is real \( \Rightarrow A_{ij} = \text{real} \times A_{ij} \)
Now (6.155) reads

\[ \overline{V} \overline{A} = \overline{A} \overline{V} \]

We can choose \( \overline{A} \) to be real.
However, the normalization of the eigenvectors is still undetermined. We choose it to be

\[ \overline{A}^T \overline{A} = \overline{I} \quad \rightarrow \quad (6.23) \]

\[ \overline{V} \overline{A} = \overline{A} \overline{V} \quad \rightarrow \quad (6.26) \]

\[ \Rightarrow \lambda_{k} = \sum_{k,l} (a^*)_{k} V_{k\ell} a_{\ell} \]

Note \( \delta_{ij} = \delta_{ii} \delta_{jj} \) and \( V_{k\ell}^* = V_{k\ell} = V_{\ell k} > 0 \)

\[ \Rightarrow \lambda_{k} = \sum_{k,l} V_{k\ell} (a^*_{k} a_{\ell}) = \sum_{k}\sum_{\ell} V_{k\ell} |a_{k\ell}|^2 \]

\[ + \sum_{k} \sum_{\ell \neq k} V_{k\ell} (a^*_{k\ell} a_{\ell}) \]

Consider \( S = \sum' a^*_{k} a_{\ell} V_{k\ell} \), \( S' \equiv \sum_{k\neq\ell} \)

\[ S = \sum' V_{k\ell} \left[ \frac{a^*_{k} a_{\ell} + a_{k\ell} a^*_{\ell}}{2} \right] \]

\[ + \sum_{k,l} V_{k\ell} \left[ |a_{k\ell} + a_{k\ell}|^2 - |a_{k\ell}|^2 - |a_{k\ell}|^2 \right] \]

\[ \Rightarrow S > 0 \]

\[ \Rightarrow \lambda_{k} > 0 \]
To summarize: We wanted to solve
\[ T \ddot{\phi} = -V \dot{\phi} \]

Now let \( \phi = \overline{A} \phi \)
\[ \Rightarrow \overline{T} \overline{A} \phi = -V \overline{A} \phi \]
\[ \Rightarrow \overline{A}^T \overline{T} \overline{A} \phi = -\overline{A}^T V \overline{A} \phi \]

Now \( (6.23) \) and \( (6.26) \) give
\[ \overline{T} \overline{A} \phi = -\overline{A} \phi \]
\[ \Rightarrow \phi_i = -\sum_j A_{ij} \phi_j = -\sum_j \lambda_{ij} \phi_j \]
\[ = -\lambda_{ii} \phi_i \]

We already proved \( \lambda_{ii} > 0 \)
Let \( \lambda_{ii} = c_i \phi_i \)
\[ \Rightarrow \phi_i = -c_i \phi_i \]
\[ \Rightarrow \phi_i = C_i \cos(c_i t + \phi_i) \]

\( C_i \) and \( \phi_i \) are integration constants.
\[ \phi(t) = \mathbb{E}(t) \]
where we define
\[ E_i = C_i \cos(c_i t + \phi_i) \]
We have now solved the problem when
\[ L = \frac{1}{2} \left[ \bar{v}^T \bar{v} - \bar{v}^T \bar{v} \right] \]

Note: → 0 We used or assumed that all \( \lambda_i = \lambda_{ii} \) were different. Hence to solve
\[ \bar{T} \bar{A} = -\bar{v} \bar{A} \bar{A}^{-1} \]
we used
\[ \text{det.} \left[ \bar{V} - \bar{A} \bar{T} \right] = 0 \]
which gave
use \( n \) distinct \( \lambda_i \) which we used to determine \((n-1)\) of the \( n, (\lambda_1, \lambda_2, \ldots, \lambda_n)\) numbers. Then we also proved reality of \( \lambda_i \) and chose the remaining unknown in \( \bar{a}_i \) to make all \( \bar{a}_i \)
real \( \Rightarrow \) \( \bar{A}^* = \bar{A} \).

Cautiön: → If all \( \lambda_i \) are not distinct
\( \Rightarrow \) above derivation gets modified.
Assume \( \lambda_1 = \lambda_2 \) then we need to use one orthogonal set \( \bar{a}_1, \bar{a}_2 \) from infinitely many possibilities. Having done that the rest of the derivation goes through.
This is the degenerate case.
\( \Phi^i, i=1, \ldots, n \) are called the normal co-ordinates since each behaves like a simple harmonic oscillator, decoupled from all the others. Show this by transforming \( L \) to \( L(\Phi^i, \dot{\Phi}^i) \).

Also, a transformation

\[
\mathbf{D} = \mathbf{C}^+ \mathbf{B} \mathbf{C}
\]

taking \( \mathbf{B} \) to \( \mathbf{D} \)

is called a congruence transformation.

Algorithm for solving small oscillations:

1. Find \( T \) & \( \Sigma \)
2. Write \( L = \frac{1}{2} \left[ \dot{\mathbf{q}}^T \mathbf{Q}^{-1} \dot{\mathbf{q}} - \mathbf{q}^T \mathbf{Q} \mathbf{q} \right] \)
3. Identify \( \mathbf{\omega} \) & \( \mathbf{\Omega} \)
4. Solve \( \text{det}(\mathbf{\Sigma} - \omega^2 \mathbf{\Omega}) = 0 \) for all \( \omega^2 \) values
5. Use \( \omega^2 \) values to find eigenvectors \( \mathbf{\alpha} \rightarrow [\mathbf{\Omega} - \omega^2 \mathbf{\Omega}] \mathbf{\alpha} = 0 \)
6. If \( \omega^2 \) are degenerate, use orthogonality of \( \mathbf{\alpha} \) vectors to get one complete set of them
7. Write the solutions in \( \mathbf{\alpha} \) time
8. Let \( \mathbf{q} = \mathbf{A} \mathbf{\alpha} \) be the general solution where \( \mathbf{\alpha} = E(t) \) has been solved
9. Use initial conditions to determine constants in \( E(t) \).