Oscillations

Consider the minimum of a potential $V(\{q_i\})$ around the point of minimum $(q_{01}, q_{02}, q_{03}, \cdots q_{0n})_{n\times 1} \equiv \bar{q}_0$

We may expand in a Taylor series as

$$V(\{q_i\}) = V(q_{01}, q_{02} + \cdots q_{0n}) + \sum_i \left(\frac{\partial V}{\partial q_i}\right)_{\bar{q}_0} (\bar{q} - \bar{q}_0)_i$$

$$+ \frac{1}{2} \sum_i \sum_j \frac{\partial^2 V}{\partial q_i \partial q_j} (\bar{q} - \bar{q}_0)_i (\bar{q} - \bar{q}_0)_j + \cdots$$

Note $\bar{q} \equiv \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix}_{n\times 1}$

At the minimum $\left(\frac{\partial V}{\partial q_i}\right)_{\bar{q}_0} = 0 \quad , \forall i$

$\therefore$ Also if we subtract the constant term $V(q_{01}, q_{02}, \cdots q_{0n})$ from the definition of V we get

$$V\{\{q_i\}\} = \sum_i \sum_j \left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_{\bar{q}_0} (q_i - q_{0i})(q_j - q_{0j})$$

neglecting higher order terms for small deviations $|\bar{q}-\bar{q}_0|$.

The kinetic energy may be written as

$$T = \sum_{i,j} \frac{m_{ij}}{2} \dot{q}_i \dot{q}_j$$

when we have no explicit time dependence in the generalized coordinates as seen from Eq (1.71).

m_{ij} are in general $m_{ij} = m_{ij}(\{q_i\})$

But to lowest order in the q_is we get

$$m_{ij}(\bar{q}) = m_{ij}(\bar{q}_0) = \text{constant}$$

Let then $T_{ij} \equiv m_{ij}(\bar{q}_0)$

$$\Rightarrow \quad T = \frac{1}{2} \dot{\bar{q}}^T \bar{\bar{T}} \dot{\bar{q}} = \frac{1}{2} \sum_i \sum_j \dot{q}_i T_{ij} \dot{q}_j$$

$$\therefore \; L = T - V = \frac{1}{2}\left[\dot{\bar{q}}^T \bar{\bar{T}} \dot{\bar{q}} - \bar{q}^T \bar{\bar{V}} \bar{q} \right] \quad \longrightarrow (6.7)$$

$$\Rightarrow \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\bar{q}}}\right) - \frac{\partial L}{\partial \bar{q}} = 0$$

$$\Rightarrow \quad \bar{\bar{T}} \ddot{\bar{q}} + \bar{\bar{V}} \bar{q} = 0 \quad \longrightarrow (6.8)$$

In writing $\overline{q}^T \overline{\overline{V}} \overline{q} = 2V$ we implicity assumed $\overline{q}_0 = 0$. This is trivially done by saying

$$\overline{q}_n = \overline{q} - \overline{q}_0 \qquad \boxed{6\text{-}3}$$

$$\dot{\overline{q}}_n = \dot{\overline{q}} \Rightarrow V = \overline{q}_n^T \overline{\overline{V}} \overline{q}_n$$

$$T = \dot{\overline{q}}_n^T \overline{\overline{T}} \overline{q}_n$$

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

Eq. (6.7) gives

$$\overline{\overline{T}} \ddot{\overline{q}} = -\overline{\overline{V}} \overline{q}$$

$$\Rightarrow \ddot{\overline{q}} = -\overline{\overline{T}}^{-1} \overline{\overline{V}} \overline{q}$$

Let $\{\lambda_k\}$ be the n non-degenerate eigenvalues and $\{\overline{a}_k\}$ be the eigenvectors of $\overline{\overline{T}}^{-1}\overline{\overline{V}}$.

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

$$\therefore \overline{\overline{T}}^{-1} \overline{\overline{V}} \overline{a}_k = \lambda_k \overline{a}_k$$

$$\overline{a}_k \equiv \begin{bmatrix} a_{k1} \\ a_{k2} \\ \vdots \\ a_{kn} \end{bmatrix}_{n \times 1} \quad \text{columns.}$$

Let $\hat{e}_k$ be unit vectors $\ni$

$$e_{ki} = \delta_{ik}$$

i.e. $\hat{e}_k = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}_{n\times 1}$, a column with all zeros but 1 at the $k^{\underline{TH}}$ row.

Define
$$\bar{\bar{A}}_{n\times n} = \sum_k \hat{e}_k \cdot \bar{a}_k^T$$

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

$$= \sum_k e_{ki} a_{kj} = \sum_k \delta_{ik} a_{kj} = a_{ij}$$

$\Rightarrow$ The $k^{\underline{TH}}$ column of $\bar{\bar{A}}$ is $\bar{a}_k$.

$$\therefore \quad \bar{\bar{T}}^{-1} \bar{\bar{V}} \bar{a}_k = \lambda_k \bar{a}_k$$

$$\Rightarrow \bar{\bar{V}} \bar{a}_k = \lambda_k \bar{\bar{T}} \bar{a}_k \longrightarrow (6.15)$$

$$\Rightarrow \bar{\bar{V}} \bar{\bar{A}} = \bar{\bar{\lambda}} \bar{\bar{T}} \bar{\bar{A}} \longrightarrow (6.15S)$$

where $\bar{\bar{\lambda}}$ is a $n\times n$ matrix which is diagonal $\Leftrightarrow$ $\lambda_{ij} = \lambda_i \delta_{ij}$

Define the Hermitian conjugate by a dagger superscript $^\dagger \ni$

$$\overline{\overline{B}}^{\dagger} \equiv \left(\overline{\overline{B}}^{T}\right)^{*} \equiv \left(\overline{\overline{B}}^{*}\right)^{T}$$

~~whe~~ where $\left(\overline{\overline{B}}^{*}\right)_{ij} \equiv \left(B_{ij}\right)^{*} \equiv B_{ij}^{*}$

where $*$ denotes complex conjugation

$(a+ib)^{*} = a-ib$ or

$\left(re^{i\theta}\right)^{*} = re^{-i\theta}$ where r is a real number.

$\overline{\overline{V}}$ and $\overline{\overline{T}}$ are real and also

$$\overline{\overline{V}}^{T} = \overline{\overline{V}} \quad \& \quad \overline{\overline{T}}^{T} = \overline{\overline{T}}$$

$$\Rightarrow \overline{\overline{V}}^{\dagger} = \overline{\overline{V}} \quad \& \quad \overline{\overline{T}}^{\dagger} = \overline{\overline{T}}$$

Eq. (6.155) gives $\overline{\overline{V}}\,\overline{\overline{A}} = \overline{\overline{\lambda}}\,\overline{\overline{T}}\,\overline{\overline{A}}$

$$\Rightarrow \overline{\overline{A}}^{\dagger}\overline{\overline{V}}\,\overline{\overline{A}} = \overline{\overline{A}}^{\dagger}\overline{\overline{\lambda}}\,\overline{\overline{T}}\,\overline{\overline{A}}$$

$$\Rightarrow \left(\overline{\overline{A}}^{\dagger}\overline{\overline{V}}\,\overline{\overline{A}}\right)^{\dagger} = \left(\overline{\overline{A}}^{\dagger}\overline{\overline{\lambda}}\,\overline{\overline{T}}\,\overline{\overline{A}}\right)^{\dagger}$$

$$\Rightarrow \overline{\overline{A}}^{\dagger}\overline{\overline{V}}\,\overline{\overline{A}} = \overline{\overline{A}}^{\dagger}\overline{\overline{T}}\,\overline{\overline{\lambda}}^{\dagger}\overline{\overline{A}}$$

$$\Rightarrow \overline{\overline{A}}^{\dagger}\overline{\overline{\lambda}}\,\overline{\overline{T}}\,\overline{\overline{A}} = \overline{\overline{T}}\,\overline{\overline{\lambda}}^{\dagger}$$

$$\Rightarrow \overline{\overline{\lambda}}\,\overline{\overline{T}} = \overline{\overline{T}}\,\overline{\overline{\lambda}}^{\dagger}$$

$\overline{\overline{\lambda}}$ is diagonal $\Rightarrow \overline{\overline{\lambda}}\,\overline{\overline{T}} = \overline{\overline{T}}\,\overline{\overline{\lambda}}$

$$\Rightarrow \overline{\overline{T}}\,\overline{\overline{\lambda}} = \overline{\overline{T}}\,\overline{\overline{\lambda}}^{\dagger} \Rightarrow \overline{\overline{\lambda}} = \overline{\overline{\lambda}}^{\dagger}$$

$\Rightarrow \overline{\overline{\lambda}}$ is real $\Rightarrow \lambda_{ij} = $ real $\forall i,j$.

Now (6.155) reads

$$\bar{\bar{V}}\bar{\bar{A}} = \bar{\bar{\lambda}}\bar{\bar{T}}\bar{\bar{A}}$$ 6-6

We can choose ∴ that $\bar{\bar{A}}$ is real
However the normalization of the eigenvectors is still undetermined. We choose it ∋

$$\bar{\bar{A}}^{\dagger}\bar{\bar{T}}\bar{\bar{A}} = \bar{\bar{I}} \longrightarrow (6.23)$$

$$\Rightarrow \bar{\bar{A}}^{\dagger}\bar{\bar{V}}\bar{\bar{A}} = \bar{\bar{\lambda}} \longrightarrow (6.26)$$

$$\Rightarrow \lambda_{ii} = \sum_{k,l} (a^{\dagger})_{ik} V_{kl} a_{li}$$

Note $\lambda_{ij} = \lambda_{ii}\delta_{ij}$ and $V_{kl}^{*} = V_{kl} = V_{lk} \geq 0$

$$\therefore \lambda_{ii} = \sum_{k,l} V_{kl}(a_{ki}^{*} a_{li}) = \sum_{k} V_{kk}|a_{ki}|^2$$

$$+ \sum_{k}\sum_{l\neq k} V_{kl}(a_{ki}^{*} a_{li})$$

Consider $S = \sum_{k,l}' a_{ki}^{*} a_{li} V_{kl}$, $\sum' \equiv \sum_{k\neq l}$

$$\therefore S = \sum_{k,l}' \frac{V_{kl}}{2}\left[a_{ki}^{*} a_{li} + a_{ki} a_{li}^{*}\right]$$

$$= \sum_{k,l}' \frac{V_{kl}}{2}\left[|a_{ki} + a_{li}|^2 - |a_{ki}|^2 - |a_{li}|^2\right]$$

$$\Rightarrow S \geq 0$$

$$\Rightarrow \lambda_{ii} \geq 0$$

To summarize: We wanted to solve

$$\overline{\overline{T}}\,\ddot{\overline{q}} = -\overline{\overline{V}}\,\overline{q} \qquad \boxed{6\text{-}7}$$

Now let $\overline{q} = \overline{\overline{A}}\,\overline{\varphi}$

$$\Rightarrow \quad \overline{\overline{T}}\,\overline{\overline{A}}\,\ddot{\overline{\varphi}} = -\overline{\overline{V}}\,\overline{\overline{A}}\,\overline{\varphi}$$

$$\Rightarrow \quad \overline{\overline{A}}^{\dagger}\,\overline{\overline{T}}\,\overline{\overline{A}}\,\ddot{\overline{\varphi}} = -\overline{\overline{A}}^{\dagger}\,\overline{\overline{V}}\,\overline{\overline{A}}\,\overline{\varphi}$$

Now (6.23) and (6.26) give

$$\overline{\overline{I}}\,\ddot{\overline{\varphi}} = -\overline{\overline{\lambda}}\,\overline{\varphi}$$

$$\Rightarrow \quad \ddot{\varphi}_i = -\sum_j \lambda_{ij}\varphi_j = -\sum \lambda_{ii}\delta_{ij}\varphi_j$$

$$= -\lambda_{ii}\varphi_i$$

We already proved $\lambda_{ii} \geq 0$

Let $\lambda_{ii} \equiv \omega_i^2$

$$\Rightarrow \qquad \ddot{\varphi}_i = -\omega_i^2\varphi_i$$

$$\Rightarrow \quad \varphi_i = C_i\cos(\omega_i t + \phi_i)$$

C_i and ϕ_i are integration constants

$\therefore \quad \overline{\varphi}(t) = \overline{E}(t)$ where we define

$$E_i \equiv C_i\cos(\omega_i t + \phi_i)$$

$$\Rightarrow \quad \bar{\bar{A}}\,\bar{\Phi}(t) = \bar{\bar{A}}\bar{E}(t)$$

$$\Rightarrow \quad \bar{q}(t) = \bar{\bar{A}}\,\bar{E}(t) = \bar{\bar{A}}\bar{E}(t)$$

We have now solved the problem when

$$L = \frac{1}{2}\left[\dot{\bar{q}}^T\,\bar{\bar{T}}\,\dot{\bar{q}} - \bar{q}^T\bar{\bar{V}}\bar{q}\right]$$

Note: → (1) We used or assumed that all $\lambda_i \equiv \lambda_{ii}$ were different. Hence to solve

$$\bar{\bar{T}}\bar{\bar{A}} = -\bar{\bar{V}}\bar{\bar{A}}\bar{\bar{\lambda}}^{-1} \text{ we used}$$

$$\det.\left[\bar{\bar{V}} - \bar{\lambda}\bar{\bar{T}}\right] = 0 \text{ which gave}$$

use n distinct λ_i which we used to determine $(n-1)$ of the n, $(a_{i1}, a_{i2}, \dots a_{in})$ numbers. Then we also proved reality of λ_i and chose the remaining ~~unk~~ unknown in $\bar{a}_i$ to make all $\bar{a}_i$ real $\Rightarrow$ $\bar{\bar{A}}^* = \bar{\bar{A}}$.

Caution: → If all λ_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.

$\bar{\bar{\varphi}}_i$, $i = 1, \ldots n$ are called the normal co-ordinates since each behaves like a simple harmonic oscillator, de-coupled from all the others.

Show this by transforming L to $L(\{\varphi_i\}, \{\dot{\varphi}_i\})$. $\boxed{6\text{-}9}$

Also a transformation

$$\bar{\bar{D}} = \bar{\bar{C}}^{\dagger} \bar{\bar{B}} \bar{\bar{C}} \text{ taking } \bar{\bar{B}} \text{ to } \bar{\bar{D}}$$

is called a congruence transformation.

Algorithm for problem solving of small oscillations

(1) Find T & V (2) Write $L = \frac{1}{2}\left[\dot{\bar{q}}^{\dagger} \bar{\bar{T}} \dot{\bar{q}} - \bar{q}^{\dagger} \bar{\bar{V}} \bar{q}\right]$

(3) Identify $\bar{\bar{T}}$ & $\bar{\bar{V}}$ (4) Solve $\det\left(\bar{\bar{V}} - \omega^2 \bar{\bar{T}}\right) = 0$ for all ω^2 values (5) Use ω^2 values to find eigenvectors $\bar{a}_i \ni \left[\bar{\bar{V}} - \omega^2 \bar{\bar{T}}\right] \bar{a} = 0$ (6) If ω^2 are degenerate use orthogonality of $\bar{a}$ vectors to get one complete set of them (7) Write the solutions in th time (8) Let $\bar{q} = \bar{\bar{A}} \bar{\varphi}$ be the general solution where $\bar{\varphi} = E(t)$ has been solved (9) Use initial conditions to determine constants in $E(t)$.