Lecture 4: THEORY OF SMALL OSCILLATIONS

The lowest order Lagrangian

\[ L \equiv T - V = \frac{1}{2}(T_{ij}\dot{\eta}_i\dot{\eta}_j - V_{ij}\eta_i\eta_j) \]  \hspace{1cm} (1)

which leads via the Lagrange’s equations to the following \( n \) equations of motion of a mechanical system near the equilibrium.

\[ T_{kj}\ddot{\eta}_j + V_{kj}\eta_j = 0 \quad (k = 1, \ldots, n). \]  \hspace{1cm} (2)

Eigenvalue Problem

These equation of motion are linear differential equations with constant coefficients, and we thus try an oscillatory solution of the form

\[ \eta_i = C a_i e^{-i\omega t} \]  \hspace{1cm} (3)

where \( C a_i \) is the complex amplitude of the oscillations for coordinate \( \eta_i \), the scaling factor \( C \) and the frequency \( \omega \) being the same for all coordinates.
\( n \) linear algebraic equations for the amplitudes \( a_i \):

\[
(V_{ij} - \omega^2 T_{ij})a_j = 0. \tag{4}
\]

These are homogeneous equations, and hence the nontrivial solution exists only if the determinant of the coefficients vanishes:

\[
\begin{vmatrix}
V_{11} - \omega^2 T_{11} & \ldots & V_{1n} - \omega^2 T_{1n} \\
\vdots & \ddots & \vdots \\
V_{n1} - \omega^2 T_{n1} & \ldots & V_{nn} - \omega^2 T_{nn}
\end{vmatrix} = 0. \tag{5}
\]
The simplified version of the general problem: the appropriate generalized coordinates are the Cartesian coordinates of the system of point particles multiplied by the square root of the particle mass (sometimes referred to as mass-weighted coordinates). The kinetic energy takes the form:

\[ T = \frac{1}{2} \ddot{\eta}^2 = \frac{1}{2}(\dot{\vec{\eta}})^2, \]  

(6)

In this case \( T_{ij} = \delta_{ij} \) and

\[ V_{ij} a_j = \lambda a_i, \]  

(7)

where \( \omega^2 = \lambda \). These equations forms the well-known eigenvalue problem of the linear algebra. It is convenient to put this problem in matrix form as

\[ V a = \lambda a, \]  

(8)

where \( V \) is \( n \times n \) matrix with elements \( V_{ij} \) and \( a \) is \( n \)-dimentional vector with components \( a_i \). This equation is referred to as the eigenvalue equations.
The values of $\lambda$ for which the equation is solvable are known as the characteristic values, or *eigenvalues* of $V$, and the vector solutions $a$ are called the *eigenvectors* of $V$. Two facts from the linear algebra:

(i) the eigenvectors of a given matrix are orthogonal to each other;

(ii) the eigenvalues of $V$ are real if $V$ is symmetrical and real.
For arbitrary symmetric and real matrix $T_{ij}$ the eigenvalue equation is rewritten in matrix form as,

$$V a = \lambda T a,$$

also stands the eigenvalue problem for a given matrix $V$. Note, that here the effect of $V$ on the eigenvector $a$ is not merely the same vector times the factor $\lambda$, but a multiple of the result of the other given matrix $T$ acting on $a$. Nevertheless, even in this general case we are in a position to show that the eigenvectors $a$ are still orthogonal, and the eigenvalues $\lambda$ are all real under some conditions imposed on $V$ and $T$. 
We can form all the eigenvectors \( a_k \) into a square matrix \( A \) with components \( a_{jk} \). Then we get one matrix equation:

\[
\tilde{A}TA = I,
\]

(10)

the transposed matrix \( A \) is obtained from \( A \) by interchanging rows and columns. This condition expresses in the matrix form orthonormality property of the eigenvectors \( a_k \), i.e. these vectors are orthogonal and of unit magnitude - but in Riemann’s space!

To show this, we must recall some facts concerning to this space. Riemann’s space, or Riemann geometry is based on the quadratic differential form in the variables \( x_1, ..., x_n \)

\[
\overline{ds}^2 = (g_{11}dx_1 + g_{12}dx_2 + g_{13}dx_3 + ... + g_{1n}dx_n)dx_1
+ (g_{21}dx_1 + g_{22}dx_2 + g_{23}dx_3 + ... + g_{2n}dx_n)dx_2

..............................................

+(g_{n1}dx_1 + g_{n2}dx_2 + g_{n3}dx_3 + ... + g_{nn}dx_n)dx_n
\]

(11)

whose coefficients, \( g_{11}, ..., g_{nn} \), are generally not constant but functions of the \( n \) variables \( x_1, ..., x_n \). These coefficients form the metric tensor \( G \) of the \( n \)-dimensional space.
Clearly for Cartesian coordinates the metric tensor is the unit matrix \( I \). In more general case of the curvilinear orthogonal coordinates (such as polar coordinates) \( G \) will be not unit but still diagonal matrix. The dot (or scalar) product of two vectors \( a \) and \( b \) in Riemann’s space is given by

\[
a \cdot b \equiv a_i g_{ik} b_k \equiv \tilde{a} G b.
\]  

(12)

If

\[
a \cdot b = \tilde{a} G b = 0,
\]  

(13)

the vectors \( a \) and \( b \) are called orthogonal. Furthermore, vector \( a \) is said to be normalized to unity if

\[
a \cdot a = \tilde{a} G a = 1.
\]  

(14)

The eigenvectors \( a_k \) are orthogonal and that they are normalized to have unit magnitude in a particular Riemann’s space for which \( T \) is the metric tensor. Note, that the kinetic energy (8) can be represented in this space as

\[
T = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j = \frac{1}{2} \tilde{\eta} T \tilde{\eta} = \frac{1}{2} \tilde{\eta} G \tilde{\eta} \equiv \frac{1}{2} \tilde{\eta} \cdot \tilde{\eta} \equiv \frac{1}{2} (\tilde{\eta})^2,
\]  

(15)
. General Solution of Equations of Motion

The trial function of the oscillatory type satisfies the equations of motion not for a single frequency but in general for a set of $n$ frequencies $\omega_k$, $k = 1, \ldots, n$. Mathematically, it means that the complete solution of the equations of motion may be written as a sum over index $k$,

$$\eta_i = C_k a_{ik} \exp^{-i\omega_k t},$$

where $C_k$ is a complex scale factor. Strictly speaking this solution must be generalized to

$$\eta_i = a_{ik}(C_k^+ \exp^{+i\omega_k t} + C_k^- \exp^{-i\omega_k t}),$$

since for each eigenvalue $\lambda_k$ (and thus for each eigenvector $a_k$) there are two frequencies $+\omega_k$ and $-\omega_k$ and accordingly two different scale factors $C_k^+$ and $C_k^-$. Nevertheless the real parts of these equations can be written in the same form

$$\eta_i = f_k a_{ik} \cos (\omega_k t + \delta_k)$$

(18)
For the determination of the constants $f_k$ and $\delta_k$ we put

$$\eta_i(0) = \text{Re} \ C_k a_{ik}$$  \hspace{1cm} (19)

Similarly, the initial value of the velocities is

$$\dot{\eta}_i(0) = \text{Im} \ C_k a_{ik} \omega_k$$  \hspace{1cm} (20)

These equations form a set of $2n$ equations from which the real and imaginary parts of the scale factors $C_k$, $\text{Re} C_k$ and $\text{Im} C_k$, may be evaluated.

In matrix relation,

$$\text{Re} \ C_l = a_{jl} T_{jk} \eta_k(0).$$  \hspace{1cm} (21)

A similar procedure with velocities gives

$$\text{Im} \ C_l = \frac{1}{\omega_l} a_{jl} T_{jk} \dot{\eta}_k(0).$$  \hspace{1cm} (22)
Normal Coordinates

The general solution for each coordinate \( \eta_i \) being a sum of simple harmonic oscillations of the frequencies \( \omega_k \) is not itself a periodic function of time. It is possible, however, to transform \( \eta_i \) to a new set of generalized coordinates that are periodic function of time. Such set of variables is known as the \textit{normal coordinates}.

The potential energy can be written as
\[
V = \frac{1}{2} \tilde{\zeta} \tilde{A} V A \tilde{\zeta} = \frac{1}{2} \tilde{\zeta} \tilde{\Lambda} \tilde{\zeta} = \frac{1}{2} \tilde{\zeta} \Lambda_{lk} \zeta_k = \frac{1}{2} \tilde{\zeta} \delta_{lk} \lambda_k \zeta_k = \frac{1}{2} \omega_k^2 \zeta_k^2.
\]
(23)

In analogous way we obtain for the kinetic energy
\[
T = \frac{1}{2} \tilde{\eta} T \tilde{\eta} = \frac{1}{2} \tilde{\zeta} \tilde{A} T A \tilde{\zeta},
\]
(24)
which can be reduced to
\[
T = \frac{1}{2} \tilde{\zeta} \cdot \dot{\zeta} = \frac{1}{2} \zeta_k^2.
\]
(25)
We notice that (i) both the potential and kinetic are sums of squares only (any cross terms vanish), and (ii) both have been diagonalized by $A$ which defines the principal axes transformation. It follows then that the principal axes transformation which we employ here is the well-known algebraic process of *simultaneous diagonalization of two quadratic forms*.

The Lagrangian in a new reference system

$$L = \frac{1}{2}(\dot{\zeta}_k \dot{\zeta}_k - \omega_k^2 \zeta_k^2), \quad (26)$$

which results in the Lagrange’s equations for $\zeta_k$

$$\ddot{\zeta}_k + \omega_k^2 \zeta_k = 0, \quad (27)$$

with an obvious solution

$$\zeta_k = C_k \exp (-i\omega_k t). \quad (28)$$

This equation demonstrates that each coordinate $\zeta_k$ is a periodic function of one of the frequencies $\omega_k$ and amplitudes $a_{ik}$. Such states are said to define the *normal modes of vibration*, and $\zeta_k$ are properly called the *normal coordinates* of the system.
Example: Triatomic Molecule

We approximate the actual complicated interatomic potential by two strings of force constant $k$, and thus take the potential energy in the form

$$V = \frac{k}{2}(x_2 - x_1 - b)^2 + \frac{k}{2}(x_3 - x_2 - b)^2. \quad (29)$$

Denoting the equilibrium position of the atoms by $x_{0i}, i = 1, 2, 3$, we have

$$x_2 - x_1 - b = x_2 - x_{02} - (x_1 - x_{01}) - b + x_{02} - x_{01} \equiv \eta_2 = x_2 - x_{02} - (x_1 - x_{01}) - b + x_{02} - x_{01} \equiv \eta_3 -$$

where we introduce new coordinates

$$\eta_i = x_i - x_{0i} \quad (31)$$

and took into account that

$$x_{02} - x_{01} = b, \quad x_{03} - x_{02} = b. \quad (32)$$

In terms of these new variables the potential is rewritten as

$$V = \frac{k}{2}(\eta_2 - \eta_1)^2 + \frac{k}{2}(\eta_3 - \eta_2)^2 =$$

$$\frac{k}{2}(\eta_1^2 + 2\eta_2^2 + \eta_3^2 - 2\eta_1\eta_2 - 2\eta_2\eta_3)$$

$$\equiv \frac{1}{2} V_{ij}\eta_i\eta_j \equiv \frac{1}{2}\tilde{\eta}V\eta. \quad (33)$$
where matrix $V$ has the form

$$V = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}. \quad (34)$$

The kinetic energy has an obvious form

$$T = \frac{m}{2} (\dot{\eta}_1^2 + \dot{\eta}_3^2) + \frac{M}{2} \dot{\eta}_2^2, \quad (35)$$

or, in matrix form

$$T = \frac{1}{2} \tilde{\eta}^T \dot{\eta}, \quad (36)$$

where $T$ is the diagonal matrix

$$T = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix}. \quad (37)$$

The characteristic equation, we obtain

$$|V - \omega^2 T| = \begin{vmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{vmatrix} = 0. \quad (38)$$

Direct evaluation of this determinant yields

$$\omega^2 (k - \omega^2 m) [\omega^2 M m - k(M + 2m)] = 0, \quad (39)$$

which immediately yields the following solutions:

$$\omega_1 = 0, \quad \omega_2 = \sqrt{\frac{k}{m}}, \quad \omega_3 = \sqrt{\frac{k}{m}(1 + \frac{2m}{M})}. \quad (40)$$
The first solution represents an example of the neutral equilibrium mentioned above: the molecule under consideration is translated along the line without any change in its potential energy - in full agreement with the corresponding equation for the first normal coordinate

\[ \ddot{\eta}_1 = 0, \]

which produces a uniform translational motion.

The second solution, \( \omega_2 \), is recognized as the frequency of oscillations for a mass \( m \) without any reference to the central mass \( M \) which remains stationary in this mode of motion. And only the third solution, \( \omega_3 \) depends on the value of the central mass which points out the participation of this mass in the motion. All these predictions are completely verified by examining the eigenvectors on the basis of the eigenvalue equation.
For the components \( a_{ij} \) with the frequency \( \omega_j \), we have
\[
\begin{align*}
(k - \omega^2 m)a_{1j} - ka_{2j} &= 0, \\
-k a_{1j} + (2k - \omega^2 M)a_{2j} - ka_{3j} &= 0, \\
-k a_{2j} + (k - \omega^2 m)a_{3j} &= 0.
\end{align*}
\] (42)

The normalization condition
\[
m(a_{1j}^2 + a_{3j}^2) + Ma_{2j}^2 = 1
\] (43)

For the first mode \( \omega_1 = 0 \), and the system immediately gives
\[
a_{11} = a_{21} = a_{31},
\] (44)
i.e. all three amplitudes are the same as it should be in the case of a pure translational motion. The values of these amplitudes are fixed by the normalization conditions which gives
\[
a_{11} = \frac{1}{\sqrt{2m + M}}, \quad a_{21} = \frac{1}{\sqrt{2m + M}} \quad (45)
\]
\[
a_{31} = \frac{1}{\sqrt{2m + M}},
\] (46)
For the second mode the amplitudes are $a_{22} = 0$ and $a_{12} = -a_{32}$, i.e. the center atom is at rest, whereas the two edge atoms vibrate exactly out of phase. The normalized values of the amplitudes are

$$a_{12} = \frac{1}{\sqrt{2m}}, \quad a_{22} = 0, \quad (47)$$

$$a_{32} = -\frac{1}{\sqrt{2m}}, \quad (48)$$

For the third mode when $(k - \omega^2 m) \neq 0$, $a_{13} = a_{33}$. Combining this with the normalization condition, we obtain

$$a_{13} = \frac{1}{\sqrt{2m(1 + \frac{2m}{M})}}, \quad a_{23} = -\frac{2}{\sqrt{2M(2 + \frac{M}{m})}}, \quad (49)$$

$$a_{33} = \frac{1}{\sqrt{2m(1 + \frac{2m}{M})}}, \quad (50)$$

In this case the two edge atoms oscillates with the same amplitudes, while the central atom vibrates out of phase with them and has a different amplitude.