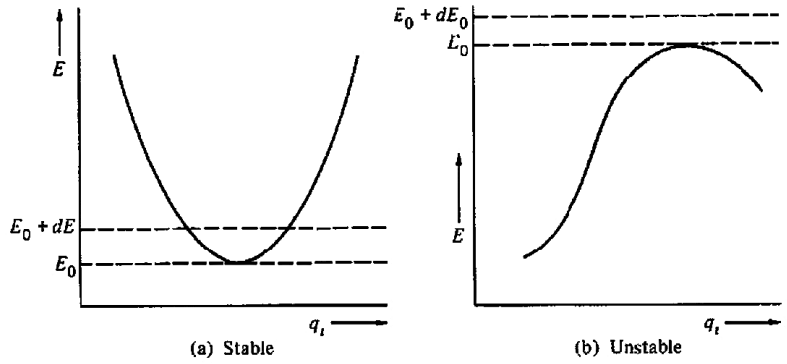
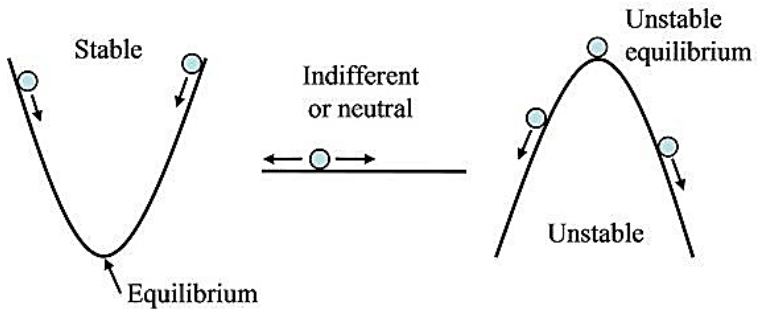
Small Oscillations

Stable and Unstable Equilibrium



If a slight displacement of the system from its position of equilibrium results only in small bounded motion about the point of equilibrium, then the system is said to be in a **stable** equilibrium. This corresponds to the minimum of potential energy because bounded motion is possible only when the potential at equilibrium is minimum. Since the potential is minimum at equilibrium, any deviation from the equilibrium position will result in an increase in potential energy and the kinetic energy would then decease (as the energy is conserved). Due to decrease in kinetic energy, the velocities would also decrease and approach zero in the course of time; the motion is thus bounded. **Examples** are a bar pendulum at rest, a suspension galvanometer at its zero position.

If a slight displacement of the system from its position of equilibrium results only in **unbounded** motion, then the system is said to be in an **unstable** equilibrium. Such a state is not characterized by minimum of potential energy. Therefore, if the system is disturbed from equilibrium by an increase in energy above the equilibrium energy, then the potential energy would decrease. Consequently, kinetic energy and hence velocities would increase infinitely with time, indicating unbound motion. A bottle standing on the edge of its mouth, a cone resting on its apex, a book placed on its edge are **examples of unstable equilibrium**.



If a system is in **neutral equilibrium**, the system will move slightly and remain at rest again instead of returning to its original position or depart far away if a slight push is exerted on the system.

Formulation of the Problem

Let us consider a conservative systems in which the potential energy is a function of position only. It will be assumed that the transformation equations defining the generalized coordinates of the system, $q_1, q_2, q_3 \dots \dots q_n$, do not involve the time explicitly. Thus, time-dependent constraints are to be excluded. The system is said to be in equilibrium when the generalized forces acting on the system vanish:

$$Q_i = -\left(\frac{\partial V}{\partial q_i}\right) = 0 \tag{1}$$

The potential energy therefore has an extremum at the equilibrium configuration of the system $q_{01}, q_{02}, q_{03} \dots \dots q_{0n}$.If the configuration is initially at the equilibrium position, with zero initial velocities $\dot{q}_n$ then the system will continue in equilibrium indefinitely.

We shall be interested in the motion of the system within the immediate neighborhood of a configuration of stable equilibrium. Since the departures from equilibrium are too small, all functions may be expanded in a Taylor series about the equilibrium, retaining only the lowest-order terms. The deviations of the generalized coordinates from equilibrium will be denoted by η_i

$$q_i = q_{0i} + \eta_i \tag{2}$$

and these may be taken as the new generalized coordinates of the motion. The Taylor series expansion of potential V about q_{0i} is

$$V(q_1, q_2, \dots \dots q_n) = V(q_{01}, q_{02}, \dots q_{0n}.) + \frac{(q_i - q_{0i})}{1!}\left(\frac{\partial V}{\partial q_i}\right)_{q_{0i}} + \frac{(q_i - q_{0i})^2}{2!}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_{q_{0i}} \eta_i\eta_j + \dots \dots \dots$$

$$\Rightarrow V(q_i) = V(q_{0i}) + \left(\frac{\partial V}{\partial q_i}\right)_{q_{0i}} \eta_i + \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_{q_{0i}} \eta_i\eta_j + \dots \dots \dots \dots$$

If we set equilibrium at 0 then,

$$V(q_i) = V(0) + \left(\frac{\partial V}{\partial q_i}\right)_0 \eta_i + \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i\eta_j + \dots \dots \dots \dots \tag{3}$$

First term $V(0)$ is a constant and has no physical significance in the sense that we can measure the potential energy with respect to any position and indeed we can choose it to be equal to zero. The first derivative of U with respect to x is zero because the curve is a minimum at x=0. The second derivative of U with respect to x, evaluated at $q_{0i} = 0$ will be a constant. Thus we retain only the first non-zero terms in the expansion is

$$V(q_i) = \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i\eta_j = \frac{1}{2}V_{ij}\eta_i\eta_j \tag{4}$$

Where the second derivatives of V have been designated by the constants V_{ij} depending only upon the equilibrium values of the q_i's. It is obvious from their definition that the V_{ij}'s are symmetrical, that is, that $V_{ij} = V_{ji}$. The V_{ij} coefficients can vanish under a variety of circumstances. Thus, the potential can simply be independent of a particular coordinate, so that equilibrium occurs at any arbitrary value of that coordinate. We speak of such cases as neutral or indifferent equilibrium.

A similar series expansion can be obtained for the kinetic energy. Since the generalized coordinates do not involve the time explicitly, the kinetic energy is a homogeneous quadratic function of the velocities

$$T = \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij} \dot{\eta}_i \dot{\eta}_j \tag{5}$$

The coefficients m_{ij} are in general functions of the coordinates q_k, but they may be expanded in a Taylor series about the equilibrium configuration:

$$m_{ij}(q_1, q_2, \ldots \ldots q_n) = m_{ij}(q_{01}, q_{02}, \ldots q_{0n}.) + \left(\frac{\partial m_{ij}}{\partial q_k}\right)_0 \eta_k + \ldots \ldots \ldots$$

$$\Rightarrow m_{ij}(q_i) = m_{ij}(0) + \left(\frac{\partial m_{ij}}{\partial q_i}\right)_0 \eta_k + \ldots \ldots \ldots \ldots$$

As eqn.(5) is already quadratic in the $\dot{\eta}_i$'s, the lowest non-vanishing approximation to T is obtained by dropping all but the first term in the expansions of m_{ij}. Denoting the constant values of the m, j functions at equilibrium by T_{ij}, we can therefore write the kinetic energy as

$$T = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j \tag{6}$$

It is again obvious that the constants T_{ij} must be symmetric, since the individual terms in eqn.(6) are unaffected by an interchange of indices. From Eqs. (4) and (6), the Lagrangian is given by

$$L = \frac{1}{2}\left(T_{ij} \dot{\eta}_i \dot{\eta}_j - V_{ij} \eta_i \eta_j\right) \tag{7}$$

Taking the η_i's as the general coordinates, the Lagrangian of Eq. (7) leads to the following n equations of motion:

$$T_{ij} \ddot{\eta}_i + V_{ij} \eta_i = 0 \tag{8}$$

These are the required equations motion.

Eigenvalue Equation and Principal Axis Transformation

The equations of motion $T_{ij} \ddot{\eta}_i + V_{ij} \eta_i = 0$ are linear differential equations with constant coefficients, of a form familiar from electrical circuit theory. We are therefore led to try an oscillatory solution of the form

$$\eta_i = C a_i e^{-i\omega t} \tag{1}$$

Here $C a_i$ gives the complex amplitude of the oscillation for each coordinate η_i the factor C being introduced for convenience as a scale factor, the same for all coordinates. It is understood of course that it is the real part of the equation of motion correspond to the actual motion. Substitution of the trial solution (1) into the equations of motion leads to the following equations for the amplitude factors:

$$V_{ij} a_i - \omega^2 T_{ij} a_i = 0 \tag{2}$$

Equations (2) constitute n linear homogeneous equations for the a_i's, and consequently can have a nontrivial solution only if the determinant of the coefficients vanishes:

$$\begin{vmatrix} V_{11}-\omega^2 T_{11} & V_{12}-\omega^2 T_{12} & \cdots \\ V_{21}-\omega^2 T_{21} & V_{22}-\omega^2 T_{22} & \cdots \\ \vdots & \vdots & \cdots \end{vmatrix} = 0 \tag{3}$$

This determinantal condition is in effect an algebraic equation of the nth degree for ω^2, and the roots of the determinant provide the frequencies for which Eq. (1) represents a correct solution to the equations of motion. Equations (2) represent a type of eigenvalue equation, for writing T_{ij} as an element of the matrix T the equations may be written

$$\boldsymbol{Va} = \lambda \boldsymbol{Ta} \tag{4}$$

Here the effect of **V** on the eigenvector **a** is not merely to reproduce the vector times the factor λ, as in the ordinary eigenvalue problem. Instead, the eigenvector is such that **V** acting on **a** produces a multiple of the result of **T** acting on **a**. The eigenvectors **a** are orthogonal. So the matrix of the eigenvectors, **a**, diagonalizes both T and V.

Let $\mathbf{a}_k$ be a column matrix representing the *k*th eigenvector, satisfying the eigenvalue equation

$$\boldsymbol{V a_k} = \lambda_k \boldsymbol{T a_k} \tag{5}$$

Assume now that the only solution to Eq. (5) involves complex λ and a_k. The adjoint equation, i.e., the transposed complex conjugate equation, for λ_l has the form

$$\boldsymbol{a_l^\dagger V} = \lambda_l \boldsymbol{Ta} \tag{6}$$

Here $\boldsymbol{a_l^\dagger}$ stands for the adjoint vector—the complex conjugate row matrix and explicit use has been made of the fact that the V and T matrices are real and symmetric. Multiply Eq. (6) from the right by λ_k and subtract the result of the similar product of Eq. (5) from the left with $\boldsymbol{a_l^\dagger}$. The left-hand side of the difference equation vanishes, leaving only

$$0 = (\lambda_k - \boldsymbol{\lambda_l^*}) \boldsymbol{a_l^\dagger T a_k} \tag{7}$$

When $l = k$, Eq. (7) becomes

$$0 = (\lambda_k - \boldsymbol{\lambda_l^*}) \boldsymbol{a_k^\dagger T a_k} \tag{8}$$

We want to prove that the matrix product is not only real but is positive definite. For this purpose, separate a_k into its real and imaginary components,

$$\boldsymbol{a_k} = \boldsymbol{\alpha_k} + \boldsymbol{i\beta_k}$$

The matrix product can then be written as

$$\boldsymbol{a_k^\dagger T a_k} = \widetilde{\boldsymbol{\alpha}}_\boldsymbol{k} \boldsymbol{T \alpha_k} + \widetilde{\boldsymbol{\beta}}_\boldsymbol{k} \boldsymbol{T \beta_k} + \boldsymbol{i}\left(\widetilde{\boldsymbol{\alpha}}_\boldsymbol{k} \boldsymbol{T \beta_k} - \widetilde{\boldsymbol{\beta}}_\boldsymbol{k} \boldsymbol{T \alpha_k}\right) \tag{9}$$

The imaginary term vanishes by virtue of the symmetry of T and therefore, as noted earlier, the matrix product is real. Further, the kinetic energy can be rewritten in terms of a column matrix $\dot{\eta}$ as

$$T = \frac{1}{2} \widetilde{\boldsymbol{\eta}} \boldsymbol{T} \dot{\boldsymbol{\eta}} \tag{10}$$

Now let us multiply now Eq. (5) by a_k from the left and solve for λ_k

$$\lambda_k = \frac{\tilde{\boldsymbol{a}}_k \boldsymbol{V} \boldsymbol{a}_k}{\tilde{\boldsymbol{a}}_k \boldsymbol{T} \boldsymbol{a}_k} \tag{11}$$

The denominator of this expression is equal to twice the kinetic energy for velocities a_{ik} and since the eigenvectors are all real, the sum must be positive definite. Similarly, the numerator is the potential energy for coordinates a_{ik}, and the condition that V be a minimum at equilibrium requires that the sum must be positive or zero. Neither numerator nor denominator can be negative, and the denominator cannot be zero, hence A is always finite and positive. (It may however be zero.) Recall that λ stands for ω^2, so that positive λ corresponds to real frequencies of oscillation. Were the potential not a local minimum, the numerator in might be negative, giving rise to imaginary frequencies that would produce an unbounded exponential increase of the in with time. Such motion would obviously be unstable.

From Eq. (7) which, in view of the reality of the eigenvalues and eigenvectors, can be written

$$(\lambda_k - \lambda_l)\tilde{\boldsymbol{a}}_l \boldsymbol{T} \boldsymbol{a}_k = 0 \tag{7*}$$

If all the roots of the secular equation are distinct, then Eq. (7*) can hold only if the matrix product vanishes for *l* not equal to k:

$$\tilde{\boldsymbol{a}}_l \boldsymbol{T} \boldsymbol{a}_k = 0, \qquad l \neq k \tag{12a}$$

It has been remarked several times that the values of the a_{ik}'s are not completely fixed by the eigenvalue equations (2). We can remove this indeterminacy by requiring further that

$$\tilde{\boldsymbol{a}}_l \boldsymbol{T} \boldsymbol{a}_k = I \tag{12b}$$

There are n such equations (12), and they uniquely fix the one arbitrary component of each of the n eigenvectors a_k. If we form all the eigenvectors a_k into a square matrix A with components a_{ik}, then the two equations (12 a and b) can be combined into one matrix equation:

$$\tilde{\boldsymbol{A}} \boldsymbol{T} \boldsymbol{A} = I \tag{13}$$

The similarity transformation of a matrix C by a matrix B was defined by the equation

$$\boldsymbol{C}' = \boldsymbol{B}\boldsymbol{C}\boldsymbol{B}^{-1}$$

We now introduce the related concept of the congruence transformation of C by A according to the relation

$$\boldsymbol{C}' = \tilde{\boldsymbol{A}}\boldsymbol{C}\boldsymbol{A} \tag{14}$$

If **A** is orthogonal, so that $\tilde{\boldsymbol{A}} = \boldsymbol{A}^{-1}$, there is no essential difference between the two types of transformation (as may be seen by denoting A^{-1} by the matrix B). Equation (13) can therefore be read as the statement that A transforms T by a congruence transformation into a diagonal matrix, in particular into the unit matrix.

If a diagonal matrix λ with elements $\lambda_{ik} = \lambda_k \delta_{lk}$ is introduced, the eigenvalue equations (5) may be written

$$V_{ij} a_{jk} = T_{ij} a_{ji} \lambda_{lk}$$

Which becomes in matrix notation

$$\boldsymbol{V}\boldsymbol{A} = \boldsymbol{T}\boldsymbol{A}\boldsymbol{\lambda} \tag{15}$$

Multiplying by $\tilde{\boldsymbol{A}}$ from the left, Eq. (15) takes the form

$$\widetilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A} = \widetilde{\boldsymbol{A}}\boldsymbol{T}\boldsymbol{A}\boldsymbol{\lambda}$$

Which by Eq. (13) reduces to

$$\widetilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A} = \boldsymbol{\lambda} \tag{16}$$

Our final equation (16) states that a congruence transformation of **V** by **A** changes it into a diagonal matrix whose elements are the eigenvalues λ_k. Eq. (16) has solutions

$$|V - \lambda I| = 0 \tag{16*}$$

In summary we can use normalized Cartesian coordinates so that $T_{ij} = \delta_{ij}$ which reduces the physics to solving

$$\widetilde{\boldsymbol{A}}\boldsymbol{A} = \boldsymbol{I} \quad and \quad \widetilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A} = \boldsymbol{V}_{diagonal}$$

or we may choose more general coordinates where $T_{ij} \neq \delta_{ij}$, even allowing $T_{ij} = T_{ji} \neq 0$ for i ≠ j, and use

$$\widetilde{\boldsymbol{A}}\boldsymbol{T}\boldsymbol{A} = \boldsymbol{I} \quad and \quad \widetilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A} = \boldsymbol{V}_{diagonal}$$

to solve the general problem.

As an example, we consider a particle of mass m with two degrees of freedom (x_1, x_2) that obeys the Lagrangian

$$L = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - \frac{1}{2}V_{ij}x_i x_j$$

where the V_{ij} are constants. The congruence transformation (16) has solutions only when Eq. (16*) is satisfied, so

$$\begin{vmatrix} V_{11} - \lambda & V_{12} \\ V_{21} & V_{22} - \lambda \end{vmatrix} = 0$$

This equation has two solutions:

$$\lambda_1 = \frac{1}{2}\left(V_{11} + V_{22} + \sqrt{(V_{11} - V_{22})^2 + 4V_{12}V_{21}}\right)$$

$$\lambda_2 = \frac{1}{2}\left(V_{11} + V_{22} - \sqrt{(V_{11} - V_{22})^2 + 4V_{12}V_{21}}\right)$$

Associated with the eigenvalues λ_i, are the eigenvectors a_{ij} that satisfy

$$a_{ij}\left(V_{ij} - \lambda_i\delta_{ij}\right) = 0 \quad and \quad a_{i1}^2 + a_{i2}^2 = 1 \quad (no\ sum\ on\ i)$$

We consider two limiting cases. The first case assumes $V_{11} > V_{22} > 0$ and $0 \neq V_{21} = V_{12} << (V_{11} - V_{22})$. We write the small quantity $\delta = [V_{12}/(V_{11} - V_{22})]$ then, to first order in δ, the eigenvalues are

$$\begin{aligned} \lambda_1 &= V_{11} + V_{22}\delta \\ \lambda_2 &= V_{11} - V_{22}\delta \end{aligned} \tag{17}$$

whose eigenvectors are, to lowest order in δ,

$$\boldsymbol{a} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 1 - \dfrac{\delta^2}{2} & -\delta + -\dfrac{\delta^3}{2} \\ \delta - \dfrac{\delta^3}{2} & 1 - \dfrac{\delta^2}{2} \end{bmatrix} \tag{18}$$

These correspond to the relations

$$a_{11} = a_{22} \quad \text{and} \quad a_{12} = -a_{21}$$

The other limiting case assumes $V_{12} > V_{22} > 0$ and $(V_{11} - V_{22}) << V_{12} = V_{21}$. We now write ε = (V11 - V22)/8V12, which is a small quantity. To first order in ε the eigenvalues are

$$\begin{aligned} \lambda_1 &= \frac{1}{2}(V_{11} + V_{22}) + V_{12} + (V_{11} - V_{22})\varepsilon \\ \lambda_2 &= \frac{1}{2}(V_{11} + V_{22}) - V_{12} - (V_{11} - V_{22})\varepsilon \end{aligned} \tag{19}$$

whose eigenvectors are, to lowest order in ε,

$$\boldsymbol{a} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{\sqrt{2}}(1 + 2\varepsilon) & -\dfrac{1}{\sqrt{2}}(1 - 2\varepsilon) \\ \dfrac{1}{\sqrt{2}}(1 - 2\varepsilon) & \dfrac{1}{\sqrt{2}}(1 + 2\varepsilon) \end{bmatrix}$$

The relations among the components of the eigenvectors ate different than in the previous example. Here $a_{12} = -a_{21}$ is slightly less than $\frac{1}{\sqrt{2}}$ while $a_{11} = a_{22}$ is slightly greater than $\frac{1}{\sqrt{2}}$. The preceding approximations looked at the behavior of the eigenvalues and eigenvectors in limiting cases.

In general, any pair of eigenvectors randomly chosen out of the infinite set of allowed vectors will not be orthogonal. Nevertheless, it is always possible to construct a pair of allowed vectors that are orthogonal, and these can be used to form the orthogonal matrix A. This processes of constructing orthogonalized eigenvectors in the case of multiple roots is completely analogous to the Gram-Schmidt method of constructing a sequence of orthogonal functions out of any arbitrary set of functions. For example, the added indeterminacy in the eigenvector components for a double root means that all of the vectors in a plane are eigenvectors. We merely choose any two perpendicular directions in the plane as being the new principal axes, with the eigenvectors in A as unit vectors along these axes.

Frequencies of Free Vibration and Normal Coordinates

If the system is displaced slightly from equilibrium and then released, the system performs small oscillations about the equilibrium with the frequencies $\omega_1, \omega_2 \ldots \ldots \omega_n$. The solutions of the secular equation are therefore often designated as the frequencies of free vibration or as the resonant frequencies of the system. The general solution of the equations of motion may now be written as a summation over an index k:

$$\eta_i = C_k a_{ik} e^{-i\omega_k t} \tag{1}$$

there being a complex scale factor C_k for each resonant frequency. It might be objected that for each solution λ_k of the secular equation there are two resonant frequencies $+\omega_k$ and $-\omega_k$. The eigenvector a_k would be

the same for the two frequencies, but the scale factors C_k^+ and C_k^- could conceivably be different. On this basis, the general solution should appear as

$$\eta_i = a_{ik}\left(C_k^+ e^{+i\omega_k t} + C_k^- e^{-i\omega_k t}\right) \tag{2}$$

Recall however that the actual motion is the real part of the complex solution, and the real part of either (1) or (2) can be written in the form

$$\eta_i = f_k a_{ik} \cos(\omega_k t + \delta_k) \tag{3}$$

where the amplitude f_k and the phase δ_k are determined from the initial conditions. The orthogonality properties of **A** greatly facilitate the determination of the scale factors C_k in terms of the initial conditions. At t = 0, the real part of Eq. (1) reduces to

$$\eta_i(0) = Re\ C_k a_{ik} \tag{4}$$

where Re stands for "real part of" Similarly, the initial value of the velocities is obtained as

$$\dot{\eta}_i(0) = Im\ C_k a_{ik} \omega_k \tag{5}$$

where Im C_k denotes the imaginary part of C_k. From these 2n equations, the real and imaginary parts of the n constants C_k may be evaluated. To solve Eq. (6.37), for example, let us first write it in terms of column matrices $\boldsymbol{\eta}$ (0) and **C**:

$$\boldsymbol{\eta}(0) = \boldsymbol{A}\ Re\ \boldsymbol{C} \tag{6}$$

If we multiply by $\widetilde{\boldsymbol{A}}\boldsymbol{T}$ from the left and use $\widetilde{\boldsymbol{A}}\boldsymbol{T}\boldsymbol{A} = \boldsymbol{I}$ we immediately obtain a solution for Re **C**:

$$\widetilde{\boldsymbol{A}}\boldsymbol{T}\boldsymbol{\eta}(0) = \widetilde{\boldsymbol{A}}\boldsymbol{T}\boldsymbol{A}\ Re\ \boldsymbol{C} = Re\ \boldsymbol{C}$$

or, taking the l^{th} component,

$$Re\ C_l = a_{lj} T_{jk} \dot{\eta}_k(0) \tag{7}$$

A similar procedure leads to the imaginary part of the scale factors as

$$Im\ C_l = \frac{1}{\omega_l} a_{lj} T_{jk} \dot{\eta}_k(0) \tag{8}$$

Equations (7) and (8) thus permit the direct computation of the complex factors C_l (and therefore the amplitudes and phases) in terms of the initial conditions and the matrices T and A.

It is possible to transform from the η_i to a new set of generalized coordinates that are all simple periodic functions of time —a set of variables known as the ***normal coordinates***. We define a new set of coordinates

$$\eta_i = a_{ij}\zeta_j \tag{9}$$

or, in terms of single column matrices $\boldsymbol{\eta}$ and $\boldsymbol{\zeta}$.

$$\boldsymbol{\eta} = \boldsymbol{A}\boldsymbol{\zeta} \tag{10}$$

The potential energy in matrix notation as

$$\boldsymbol{V} = \frac{1}{2}\tilde{\boldsymbol{\eta}}\boldsymbol{V}\boldsymbol{\eta} \tag{11}$$

Now, the single-row transpose matrix $\tilde{\boldsymbol{\eta}}$ is related to $\tilde{\zeta}$ by the equation

$$\tilde{\boldsymbol{\eta}} = \widetilde{\boldsymbol{A}\boldsymbol{\zeta}} = \tilde{\boldsymbol{\zeta}}\tilde{\boldsymbol{A}} \tag{12}$$

so that the potential energy can be written also as

$$\boldsymbol{V} = \frac{1}{2}\tilde{\boldsymbol{\zeta}}\tilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A}\boldsymbol{\zeta}$$

But **A** diagonalizes **V** by a congruence transformation and the potential energy therefore reduces simply to

$$\boldsymbol{V} = \frac{1}{2}\tilde{\boldsymbol{\zeta}}\boldsymbol{\lambda}\boldsymbol{\zeta} = \frac{1}{2}\omega_k^2\zeta_k^2 \tag{13}$$

The kinetic energy has an even simpler form in the new coordinates. Since the velocities transform as the coordinates, T transforms to

$$\boldsymbol{T} = \frac{1}{2}\tilde{\dot{\boldsymbol{\zeta}}}\tilde{\boldsymbol{A}}\boldsymbol{V}\boldsymbol{A}\dot{\boldsymbol{\zeta}}$$

which reduces to

$$\boldsymbol{T} = \frac{1}{2}\tilde{\dot{\boldsymbol{\zeta}}}\dot{\boldsymbol{\zeta}} = \frac{1}{2}\dot{\zeta}_i\dot{\zeta}_i \tag{14}$$

The equations of motion share in the simplification resulting from their use. The new Lagrangian is

$$L = \frac{1}{2}\left(\dot{\zeta}_i\dot{\zeta}_i - \omega_k^2\zeta_k^2\right)$$

so that the Lagrange equations for ζ_k are

$$\ddot{\zeta}_k + \omega_k^2\zeta_k = 0 \tag{15}$$

Equations (15) have the immediate solutions

$$\zeta_k = C_k e^{-i\omega_k t}$$

Each of the new coordinates is thus a simply periodic function involving only one of the resonant frequencies. As mentioned earlier, it is therefore customary to call the ζ's the ***normal coordinates*** of the system.

Each normal coordinate corresponds to a vibration of the system with only one frequency, and these component oscillations are spoken of as the ***normal modes of vibration***. All of the particles in each mode vibrate with the same frequency and with the same phase; the relative amplitudes being determined by the matrix elements a_{ij}.

Harmonics of the fundamental frequencies are absent in the complete motion essentially because of the stipulation that the amplitude of oscillation be small. We are then allowed to represent the potential as a quadratic form, which is characteristic of simple harmonic motion. The normal coordinate transformation emphasizes this point.

Free Vibrations of a Linear Triatomic Molecule

To illustrate the technique for obtaining the resonant frequencies and normal modes, we shall consider in detail a model based on a linear symmetrical tri-atomic molecule. In the equilibrium configuration of the molecule, two atoms of mass in are symmetrically located on each side of an atom of mass M (Fig. 1). All three atoms are on one straight line, the equilibrium distances apart being denoted by b. For simplicity, we shall first consider only vibrations along the line of the molecule, and the actual complicated interatomic potential will be approximated by two springs of force constant k joining the three atoms. There are three obvious coordinates marking the position of the three atoms on the line. In these coordinates, the potential energy is

$$V = \frac{1}{2}k(x_2 - x_1 - b)^2 + \frac{1}{2}k(x_3 - x_2 - b)^2 \tag{1}$$

We now introduce coordinates relative to the equilibrium positions:

$$\eta_i = x_i - x_{0i}$$

Where

$$x_{02} - x_{01} = b = x_{03} - x_{02}$$

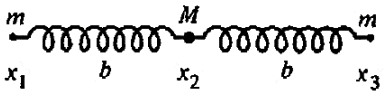


Fig.1: Model of a linear symmetrical triatomic molecule.

The potential energy then reduces to

$$V = \frac{1}{2}k\{x_2 - x_1 - (x_{02} - x_{01})\}^2 + \frac{1}{2}k\{x_3 - x_2 - (x_{03} - x_{02})\}^2$$

$$= \frac{1}{2}k(\eta_2 - \eta_1)^2 + \frac{1}{2}k(\eta_3 - \eta_2)^2$$

$$= \frac{1}{2}k({\eta_2}^2 - 2\eta_1\eta_2 + {\eta_1}^2 + {\eta_3}^2 - 2\eta_2\eta_3 + {\eta_2}^2)$$

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

$$2V = [\eta_1 \quad \eta_2 \quad \eta_3]\begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix}\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}$$

Hence, the V tensor has the form

$$V = (V_{ij}) = \begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix} \tag{2}$$

The kinetic energy has an even simpler form:

$$T = \frac{1}{2}m(\dot{\eta_1}^2 + \dot{\eta_3}^2) + \frac{1}{2}M\dot{\eta_2}^2$$

$$\Rightarrow 2T = [\dot{\eta}_1 \quad \dot{\eta}_2 \quad \dot{\eta}_3] \begin{bmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{bmatrix} \begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \\ \dot{\eta}_3 \end{bmatrix}$$

$$\Rightarrow T = (T_{ij}) = \begin{bmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{bmatrix} \tag{3}$$

so that the T tensor is diagonal.

$$\omega^2 T = \begin{bmatrix} \omega^2 m & 0 & 0 \\ 0 & \omega^2 M & 0 \\ 0 & 0 & \omega^2 m \end{bmatrix} \tag{4}$$

Combining these two tensors,

$$V - \omega^2 T = \begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix} - \begin{bmatrix} \omega^2 m & 0 & 0 \\ 0 & \omega^2 M & 0 \\ 0 & 0 & \omega^2 m \end{bmatrix} = 0$$

$$\begin{bmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{bmatrix} = 0$$

$$(k - \omega^2 m)\{(2k - \omega^2 M)(k - \omega^2 m) - k^2\} + k\{-k(k - \omega^2 m)\} = 0$$

$$(k - \omega^2 m)[(2k - \omega^2 M)(k - \omega^2 m) - 2k^2] = 0$$

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

$$\omega^2(k - \omega^2 m)[-2km - Mk + M\omega^2 m] = 0$$

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

Which has roots

$$\omega_1 = 0; \qquad \omega_2 = \sqrt{\frac{k}{m}}\,; \qquad \omega_3 = \sqrt{\frac{k}{m}\left(\frac{2m}{M} + 1\right)}$$

The first eigenvalue, $\omega_1 = 0$, may appear somewhat surprising and even alarming at first sight. Such a solution does not correspond to an oscillatory motion at all, for the equation of motion for the corresponding normal coordinate is

$$\ddot{\zeta_1} = 0$$

Which produces a uniform translational motion. But this is precisely the key to the difficulty. The vanishing frequency arises from the fact that the molecule may be translated rigidly along its axis without any change in the potential energy, an example of neutral equilibrium mentioned previously. Since the restoring force against such motion is zero, the effective "frequency" must also vanish. We have made the assumption that the molecule has three degrees of freedom for vibrational motion, whereas in reality one of them is a rigid body degree of freedom.

Normal Coordinates and Normal Modes

In the principal axis transformation we consider a new set of coordinates. Each of the new coordinates is simply a periodic function involving only one of the resonant frequencies which are the ***normal coordinates*** of the system.

A normal mode of an oscillating system is a pattern of motion in which all parts of the system move sinusoidally with the same frequency and with a fixed phase relation. The free motion described by the normal modes takes place at the fixed frequencies. These fixed frequencies of the normal modes of a system are known as its natural frequencies or resonant frequencies. A physical object, such as a building, bridge, or molecule, has a set of normal modes and their natural frequencies that depend on its structure, materials and boundary conditions. When relating to music, normal modes of vibrating instruments (strings, air pipes, drums, etc.) are called "harmonics" or "overtones".

Forced Vibrations and the Effect of Dissipative Forces

When the system is set into oscillation by an external driving force that continues to act on the system after t = 0 then the vibration is called the forced vibration. The frequency of such a forced oscillation is then determined by the frequency of the driving force and not by the resonant frequencies. Though, the normal modes are of great importance in obtaining the amplitudes of the forced vibration, and the problem is greatly simplified by use of the normal coordinates obtained from the free modes.

If $\boldsymbol{F_j}$ is the generalized force corresponding to the coordinate η_j then the generalized force Q, for the normal coordinate Q_i is

$$Q_i = a_{ij} F_i \tag{1}$$

The equations of motion when expressed in normal coordinates now become

$$\ddot{\zeta}_i + \omega^2 \zeta_i = Q_i \tag{2}$$

Equations (2) are a set of n inhomogeneous differential equations that can be solved only when we know the dependence of Q, on time. While the solution will not be as simple as in the free case, note that the normal coordinates preserve their advantage of separating the variables, and each equation involves only a single coordinate.

Frequently, the driving force varies sinusoidally with time. In an acoustic problem, for example, the driving force might arise from the pressure of a sound wave impinging on the system, and Qi then has the same frequency as the sound wave. Or, if the system is a polyatomic molecule, a sinusoidal driving force is present

if the molecule is illuminated by a monochromatic light beam. Each atom in the molecule is then subject to an electromagnetic force whose frequency is that of the incident light. Even where the driving force is not sinusoidal with a single frequency, it can often be considered as built up as a superposition of such sinusoidal terms. Thus, if the driving force is periodic, it can be represented by a Fourier series; other times, a Fourier integral representation is suitable. Since Eqs. (2) are linear equations, its solutions for particular frequencies can be superposed to find the complete solution for given Q_i.

It is therefore of general interest to study the nature of the oscillations when the force Q, can be written as

$$Q_i = Q_{0i}\cos(\omega t + \delta_i) \tag{3}$$

Where ω is the angular frequency of an external force. The equations of motion now appear as

$$\ddot{\zeta}_i + \omega^2\zeta_i = Q_{0i}\cos(\omega t + \delta_i) \tag{4}$$

A complete solution of Eq. (4) consists of the general solution to the homogeneous equation (that is, the free modes of vibration) plus a particular solution to the inhomogeneous equation. By a proper choice of initial conditions, the superimposed free vibrations can be made to vanish, centering our interest on the particular solution of Eqs. (4) that will obviously have the form 4

$$\zeta_i = B_i\cos(\omega t + \delta_i) \tag{5}$$

Here the amplitudes B_i are determined by substituting the solution in Eqs. (5):

$$B_i = \frac{Q_{0i}}{\omega_i^2 - \omega^2} \tag{6}$$

The complete motion is then

$$\eta_j = a_{ji}\zeta_i = \frac{a_{ji}\,Q_{0i}\cos(\omega t + \delta_i)}{\omega_i^2 - \omega^2} \tag{7}$$

Thus, the vibration of each particle is again, composed of linear combinations of the normal modes, but now each normal oscillation occurs at the frequency of the driving force.

Two factors determine the extent to which each normal mode is excited:

One is the amplitude of the generalized driving force, Q_{0i}. If the force on each particle has no component in the direction of vibration of some particular normal mode, then obviously the generalized force corresponding to the mode will vanish and Q0, will be zero. An external force can excite a normal mode only if it tends to move the particles in the same direction as in the given mode.

The second factor is the closeness of the driving frequency to the free frequency of the mode. As a consequence of the denominators in Eq. (7), the closer ω approaches to any ω_I, the stronger will that mode be excited relative to the other modes. Indeed, Eq. (7) apparently predicts infinite amplitude when the driving frequency agrees exactly with one of the ω_i's - the familiar phenomenon of resonance. Note that the oscillations are in phase with the driving force when the frequency is less than the resonant frequency, but that there is a phase change of at in going through the resonance.

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Our discussion has been unrealistic in that the absence of dissipative or frictional forces has been assumed. In many physical systems, these forces, when present, are proportional to the particle velocities and can therefore be derived from a dissipation function $\mathcal{F}$. Let us first consider the effects of frictional forces on the free modes of vibration. From its definition, $\mathcal{F}$ must be a homogeneous quadratic function of the velocities:

$$\mathcal{F} = \frac{1}{2}\mathcal{F}_{ij}\dot{\eta}_i\dot{\eta}_j \tag{8}$$

The coefficients $\mathcal{F}_{ij}$ are clearly symmetric, $\mathcal{F}_{ij} = \mathcal{F}_{ji}$, and in general will be functions of the coordinates. Since we are concerned with only small vibrations about equilibrium, it is sufficient to expand the coefficients about equilibrium and retain only the first, constant term, exactly as was done for the kinetic energy. In future applications of Eq. (8), we shall take $\mathcal{F}_{ij}$ as denoting these constant factors. Recall that $2\mathcal{F}$ is the rate of energy dissipation due to the frictional forces. The dissipation function $\mathcal{F}$ therefore can never be negative. The complete set of Lagrange equations of motion now become

$$T_{ij}\ddot{\eta}_j + \mathcal{F}_{ij}\dot{\eta}_j + V_{ij}\eta_j = 0 \tag{9}$$

Clearly in order to find normal coordinates for which the equations of motion would be decoupled, it is necessary to find a principal axis transformation that simultaneously diagonalizes the three quadratic forms T, V, and $\mathcal{F}$ As was shown above, this is not in general possible; normal modes cannot usually be found for any arbitrary dissipation function.

There are however some exceptional cases when simultaneous diagonalization is possible. For example, if the frictional force is proportional both to the particle's velocity and its mass, then F will be diagonal whenever T is. When such simultaneous diagonalization is feasible, then the equations of motion are decoupled in the normal coordinates with the form (10)

$$\ddot{\zeta}_i + \mathcal{F}_i\dot{\zeta}_i + \omega^2\zeta_i = 0$$

Here the $\mathcal{F}_i$'s are the nonnegative coefficients in the diagonalized form of $\mathcal{F}$ when expressed in terms of ζ_i. Being a set of linear differential equations with constant coefficients, Eqs. (10) may be solved by functions of the form

$$\zeta_i = C_i e^{-i\omega_i' t} \tag{11}$$

where ω_i' satisfies the quadratic equation

$$\omega_i'^2 + i\omega_i'\mathcal{F}_i - \omega_i^2 = 0 \tag{12}$$

Equation (6.70) has the two solutions

$$\omega_i' = \pm\sqrt{\omega_i^2 - \frac{\mathcal{F}_i^2}{4}} - i\frac{\mathcal{F}_i}{2} \tag{13}$$

The motion is therefore not a pure oscillation, for ω_i' is complex. It is seen from Eq. (13) that the imaginary part of ω_i' results in a factor $\exp(-\frac{\mathcal{F}_i t}{2})$, and by reason of the nonnegative nature of of the $\mathcal{F}_i$'s, this is always an exponentially decreasing function of time. The presence of a damping factor due to the friction is hardly unexpected. As the particles vibrate, they do work against the frictional forces, and the energy of the system (and hence the vibration amplitudes) must decrease with time. The real part of Eq. (13) corresponds to the oscillatory factor in the motion; note that the presence of friction also affects the frequency of the vibration.

However, if the dissipation is small, the squared term in I; may be neglected, and the frequency of oscillation reduces to the friction-free value.

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