CHAPTER I

INTRODUCTION

Vibtration Theory and Normal Coordinates[1]

Many problems of mechanics are concerned with the vibrations of a system of particles. By a vibration we mean the oscillations of a system when it is slightly disturbed from a position of stable equilibrium. In such a motion no coordinate ever departs by a large amount from the value it would have if the system were in the equilibrium position. It is convenient in these problems to choose a system of coordinates such that all the q_i's vanish at the point of equilibrium; then all the q_i's will remain small throughout the motion.

If we were to express the coordinates of each particle by a set of rectangular coordinates with the origin at the equilibrium position of the particle, the kinetic energy of the system would be

$$T = \frac{1}{2} \sum_i m_i \left(\frac{dx_i}{dt}\right)^2 \qquad \text{.............(1.1)}$$

Usually a more general coordinate system would be used; the kinetic energy of the system in generalized coordinates is of the form

---

[1] Eyring, Henry., Walter, John., and Kimball, George E. *Quantum Chemistry*. (New York: John Wiley and Sons, Inc., 1944), pp. 16-20.

$$T = \frac{1}{2} \sum_i \sum_j a_{ij} \frac{dq_i}{dt} \frac{dq_j}{dt} \quad \ldots\ldots\ldots\ldots(1.2)$$

where the a_{ij}'s are functions of the q_i's, but for small vibrations it will be a sufficiently good approximation to regard the a_{ij}'s as constants, with the value they have at the equilibrium position. The potential energy may be expanded in a Taylor's series in the q's about the point of equilibrium:

$$V = V_o + \sum_i \left(\frac{\partial V}{\partial q_i}\right)_o q_i + \Sigma_i \Sigma_j \tfrac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_o q_i q_j + \ldots\ldots(1.3)$$

where the derivatives are evaluated at $q_i = 0$, the position of equilibrium. The constant term V_o is arbitrary, and so for the sake of simplicity we take it to be zero. Since $q_i = 0$ is a point of equilibrium, V must be a minimum at this point, so that $\left(\frac{\partial V}{\partial q_i}\right)_o = 0$. If we denote the constant $\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_o$ by b_{ij}, we may therefore represent V approximately by

$$V = \frac{1}{2} \sum_i \sum_j b_{ij} q_i q_j \quad \ldots\ldots\ldots\ldots(1.4)$$

By substituting in Lagrange's equations,

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{q}_j} - \frac{\partial}{\partial q_j} (T-V) = 0 \quad \ldots\ldots\ldots\ldots(1.5)$$

Lagrange's equations for the system are then

$$\sum_j a_{ij} \frac{d^2 q_j}{dt^2} + \sum_j b_{ij} q_j = 0 \quad \ldots\ldots\ldots\ldots(1.6)$$

If the system has F degrees of freedom, there are F of these differential equations corresponding to i = 1,2,... F. In order to solve these equations let us try to find a set of constants c_i such that, if each equation of the set is multiplied by c_i and the results added together, the new equations will be of the form

$$\frac{d^2Q}{dt^2} + \lambda Q = 0 \qquad \text{............(1.7)}$$

where Q is an expression of the form

$$Q = \sum_j h_j q_j \qquad \text{............(1.8)}$$

The equations which must be satisfied in order to obtain this result are

$$\sum_i c_i a_{ij} = \frac{1}{\lambda} \sum_i c_i b_{ij} = h_j \qquad \text{............(1.9)}$$

The equations given by the equality sign on the left are just sufficient to determine the c_i's; the remaining equations will then give the h_j's.

If we write the left-hand equation in the form

$$\sum_i (\lambda a_{ij} - b_{ij}) c_i = 0 \qquad \text{............(1.10)}$$

It is seen that one solution is $c_i = 0$. This is the only solution unless the determinant of the coefficients vanishes, that is

$$|\lambda a_{ij} - b_{ij}| = 0 \qquad \text{............(1.11)}$$

This equation may be satisfied if we choose λ properly. Let λ_1 be one of the F roots of this equation. Then the equations

$$\sum_i (\lambda_1 a_{ij} - b_{ij}) c_i = 0 \qquad \ldots\ldots\ldots\ldots(1.12)$$

have a set of non-vanishing solutions for the c_i's, which are unique except for one arbitrary constant factor.

When this set of d_i's has been determined, the h_i's are fixed by equation (1.9).

Let these be denoted by $h_i^{(1)}$ and the corresponding Q by Q_1. In the same way each of the other roots of (1.11) gives a set of h_i's which in turn determines a possible Q, so that we arrive at a set of F Q's, each of which satisfies the equation

$$\frac{d^2Q_i}{dt^2} + \lambda_i Q_i = 0 \quad (i = 1,2,\ldots.F) \qquad \ldots\ldots\ldots\ldots(1.13)$$

If we regard the Q's as a new set of coordinates, these equations are just Lagrange's equations in the new coordinates. Because of the simple form of these equations the Q's are known as the normal coordinates of the system.

In terms of the normal coordinates, the kinetic and potential energies have the simple form:

$$T = \tfrac{1}{2} \sum_i \left(\frac{dQ_i}{dt}\right)^2 \qquad V = \tfrac{1}{2} \sum_i \lambda_i Q_i^2 \qquad \ldots\ldots\ldots\ldots(1.14)$$

If the equilibrium is stable, then all the λ_i's $(\lambda_i = \frac{\partial^2 V}{\partial Q_i^2})$ are real and positive. But for the positive λ's it is easily seen that the solution of the equation (1.13) is

$$Q_i = A_i \cos(\sqrt{\lambda_i}\, t + \epsilon_i) \qquad \text{..........(1.15)}$$

where A_i and ϵ_i are arbitary constants

If the solution is desired in terms of the original coordinates, the q_i's must be expressed in terms of the Q_i's by solving simultaneously the equations defining the Q_i's. Suppose that the result is

$$q_i = \sum_j g_{ij} Q_j \qquad \text{............(1.16)}$$

Then the equations of motion are

$$q_i = \sum_j g_{ij} A_j \cos(\sqrt{\lambda_j}\, t + \epsilon_j) \qquad \text{............(1.17)}$$

If all the A_j's are zero except one, then each q_i varies sinusoidally with time, each with the same phase. Such a motion is called a normal mode of vibration of the system. Corresponding to such a mode of vibration there is a definite frequency given by $\nu_j = \frac{\sqrt{\lambda_j}}{2\pi}$. The most general vibration of the system can be regarded as a superposition of the various normal modes, with arbitary amplitudes and phases.

If the equilibrium is unstable, the above formal treatment can still be carried out. In this case, however, at least one of the λ's is real and negative, so that the corresponding frequency is imaginary. The motion then is not sinusoidal, since the Q corresponding to the negative λ will be an exponentially increasing function of the time.

<u>Example</u> Three springs, whose force constants are k, 2k, and k, are joined in a straight line, and the ends of the system are fixed. The joints between the springs are balls of mass m. Determine the motion if the balls are set vibrating in the line of the springs.

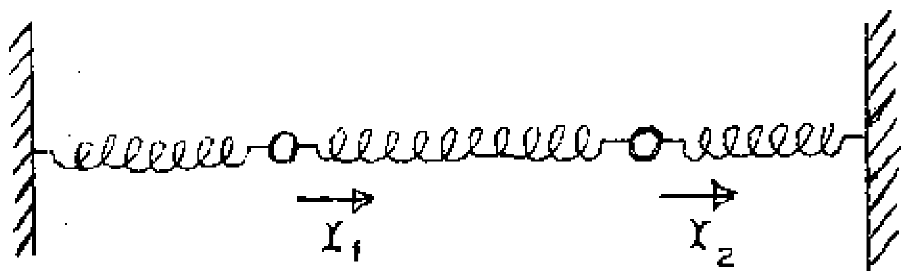

Figure 1. **Displacement coordinates x_1 and x_2.**

Let the displacement of the first ball from its equilibrium position be x_1 and that of the second ball x_2. The changes in length of the three springs are then $x_1, x_2-x_1, -x_2$, so that the potential energy of the system is

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

$$= \frac{3}{2} k x_1^2 - 2k x_1 x_2 + \frac{3}{2} k x_2^2 \qquad \ldots\ldots\ldots\ldots(1.18)$$

If we consider the springs to have zero mass, the kinetic energy is

$$T = \frac{m}{2}\left[\left(\frac{dx_1}{dt}\right)^2 + \left(\frac{dx_2}{dt}\right)^2\right] \qquad \text{..........(1.19)}$$

Lagrange's equations of motion are therefore

$$m\frac{d^2x_1}{dt^2} + 3\,k\,x_1 - 2k\,x_2 = 0$$

$$m\frac{d^2x_2}{dt^2} - 2k\,x_1 + 3k\,x_2 = 0 \qquad \text{..........(1.20)}$$

If we multiply the first of these equations by c_1 and the second by c_2 and add, we obtain

$$mc_1\frac{d^2x_1}{dt^2} + mc_2\frac{d^2x_2}{dt^2} + (3kc_1 - 2kc_2)x_1$$

$$+ (-2kc_1 + 3kc_2)\,x_2 = 0 \qquad \text{..........(1.21)}$$

In order that this be of the form (1.7) we must have

$$mc_1 = \frac{1}{\lambda}(3kc_1 - 2kc_2) = h_1$$

$$mc_2 = \frac{1}{\lambda}(-2kc_1 + 3kc_2) = h_2 \qquad \text{..........(1.22)}$$

There will be a non-trivial solution for c_1 and c_2 only if

$$\begin{vmatrix} \lambda m - 3k & 2k \\ 2k & \lambda m - 3k \end{vmatrix} = 0 \qquad \text{..........(1.23)}$$

The roots of the determinant are $\lambda_1 = \frac{5k}{m}$; $\lambda_2 = \frac{k}{m}$. Substituting λ_1 in equation (1.22) gives $c_1 = -c_2$. Hence if we take c_1, which is arbitrary, to be 1, c_2 must be -1, and

$$Q_1 = h_1^{(1)} x_1 + h_2^{(1)} x_2 = m x_1 - m x_2 \quad ....(1.24)$$

In the same way we find for Q_2 the value

$$Q_2 = m x_1 + m x_2 \quad ....(1.25)$$

The equations of motion in the new coordinates are

$$\frac{d^2Q_1}{dt^2} + \frac{5k}{m} Q_1 = 0$$

$$\frac{d^2Q_2}{dt^2} + \frac{k}{m} Q_2 = 0 \quad ....(1.26)$$

The first normal mode is that in which $Q_2 = 0$, that is, $x_1 + x_2 = 0$. In this normal mode the balls move in opposite directions with a frequency $\frac{1}{2\pi}\sqrt{\frac{5k}{m}}$.

In the second normal mode $x_1 = x_2$; the balls move in the same direction with a frequency $\frac{1}{2\pi}\sqrt{\frac{k}{m}}$.