UNIT-1
Equations of Motion

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1.0 Objectives

In this chapter we shall focus upon the following topics

- Generalized coordinates
- Lagrangian for a system
- The principle of least action
- Galileo's relativity principle

1.1 Introduction

Classical mechanics deals with the motion of physical bodies at the macroscopic level. Galileo and Newton laid its foundation. However if the system is subject to external constraints, solving the equation of motion may be difficult

and sometimes it may be difficult even to formulate them. To circumvent these difficulties two different methods, Lagrange's and Hamilton's formulations, have been developed. Before going over to these procedures, we have to understand certain terms such as constraints, generalized coordinates etc. In this chapter we start from the fundamental principle of mechanics viz. the principle of least action and deduce Lagrange's equation of motion. We make use of Lagrange's equation in solving complicated problem from the point of Newtonian mechanics.

1.2 Generalized Coordinates

Mechanics and its domain;

Mechanics is the study of motion of material bodies e.g., the motion of celestial bodies, path of a projectile, motion of a space-satellite . *Classical mechanics now-a-days has come into wide use to denote that part of mechanics where the objects in question are neither too big so that a close agreement between theory and experiment is desirable, nor too small interacting objects , more precisely , systems on an atomic scale.* These extreme cases are dealt within general theory of relativity and quantum mechanics , respectively.

Generalized co-ordinates

One of the fundamental concepts of mechanics is that of a *particle* or sometimes called a *material point*. By this we mean a body whose dimensions may be neglected in describing its motion. The possibility of so doing depends, of course, on the conditions of the problem concerned. For example, the planets may be regarded as particles in describing their motion about the Sun, but not in considering their rotation about their axes.

The position of a particle in space is defined by its radius vector $\boldsymbol{r}$, whose components are the Cartesian co-ordinates x, y, z. The derivative $v = d\,r\,/\,d\,t$ of $\boldsymbol{r}$ with respect to time is called the velocity of the particle, and the second derivative $v = d^2\,r\,/\,d\,t^2$ is its acceleration. In what follows we shall, as is customary, denote differentiation with respect to time by placing a dot above a letter: $v = \dot{r}$.

To define the position of a system of $\boldsymbol{N}$ particles in space, it is necessary to specify $\boldsymbol{N}$ radius vectors, i.e. $\boldsymbol{3N}$ co-ordinates. ***The number of independent quantities which must be specified in order to define uniquely the position of any system is***

called the number of degrees of freedom; here, this number is $3N$. These quantities need not be the Cartesian co-ordinates of the particles, and the conditions of the problem may render some other choice of co-ordinates more convenient. ***Any s quantities $q_1, q_2, ...q_s$ which completely define the position of a system with s degrees of freedom are called generalized co-ordinates of the system, and the derivatives $\dot{q}_i$ are called its generalized velocities.*** For short, we shall often conventionally denote by q the set of all the co-ordinates $q_1, q_2, ...q_s$ and similarly by $\dot{q}$ the set of all the velocities.

How to define the mechanical state of the system?

When the values of the generalized co-ordinates are specified, however, the " mechanical state"

of the system at the instant considered is not yet determined in such a way that the position of the system at the subsequent instants can be predicted. For given values of the co-ordinates , the system can have any velocities, and these affect the position of the system after an infinitesimal time interval *dt*.

*If all the co-ordinates and velocities are simultaneously specified, it is known from experience that the state of the system is completely determined and its subsequent motion can, in principle, be calculated***.** Mathematically, this means that, if all the co-ordinates q and velocities $\dot{q}$ are given at some instant, the accelerations $\ddot{q}$ at that instant are uniquely defined.

The equations of motion:

The relations between the accelerations, velocities and co-ordinates are called the *equations of motion*. They are second-order differential equations for the function $q(t)$, and their integration makes possible, in principal, the determination of these functions and so the path of the system.

1.3 The Principle of Least Action

The most general formulation of the law governing the motion of mechanical systems is the ***principle of least action*** **or** ***Hamilton's principle***, according to which every mechanical system is characterized by a definite function $L(q_1, q_2, ... q_s, \dot{q}_1, \dot{q}_2, ... \dot{q}_s, t)$, or in short $L(q, \dot{q}, t)$, and the motion of the system is such that a certain condition is satisfied.

Let the system occupy, at the instants t_1 and t_2, positions defined by two sets of values of the co-ordinates, $q^{(1)}$ and $q^{(2)}$. Then the condition is that the system moves between these positions in such a way that the integral

$$\boxed{S = \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt} \tag{1}$$

takes the least possible value. The function L is called the *Lagrangian* of the system concerned, and the integral (1) is called the ***action***.

Derivation of the Lagrange's equations

We now derive the differential equations which solve the problem of minimizing the integral (1). For simplicity, we shall first assume that the system has only one degree of freedom, so that only one function $q(t)$ has to be determined.

Let $q = q(t)$ be the function for which S is a minimum. This means that S is increased when $q(t)$ is replaced by any function of the form

$$q(t) + \delta q(t) \tag{2}$$

where $\delta q(t)$ is a function which is small everywhere in the interval of time from $t = t_1$ to $t = t_2$; $\delta q(t)$ is called a ***variation*** of the function $q(t)$. Since, for $t = t_1$ and for $t = t_2$, all the functions (2) must take the values $q^{(1)}$ and $q^{(2)}$ respectively , it follows that

$$\delta q(t_1) = \delta q(t_2) = 0 \tag{3}$$

The change in S when q is replaced by $q + \delta q$ is

$$\int_{t_1}^{t_2} L(q + \delta q, \dot{q} + \delta \dot{q}, t)\, dt - \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt .$$

When this difference is expanded in powers of δq and $\delta \dot{q}$ in the integrand, the leading terms are of the first order. The necessary condition for S to have a minimum (or, in general , an extremum) is that these terms (called the *first variation*, or simply the *variation* , of the integral) should be zero. Thus the principle of least action may be written in the form

$$\boxed{\delta S = \delta \int_{t_1}^{t_2} L\,(q\ ,\dot{q}\ ,t)\,dt = 0}\ , \tag{4}$$

or, effecting the variation,

$$\int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q}\,\delta q + \frac{\partial L}{\partial \dot{q}}\,\delta \dot{q}\right) dt = 0\ .$$

Since $\delta\,\dot{q} = \delta\,\frac{d}{dt}(q) = \frac{d}{dt}(\delta\,q\,(t))$, we obtain, on integrating the second term by parts,

$$\delta S = \left[\frac{\partial L}{\partial q}\,\delta q\right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{\frac{\partial L}{\partial q} \quad \frac{d}{dt}\,\frac{\partial L}{\partial \dot{q}}\right\} \delta q\,dt = 0 \tag{5}$$

The conditions (3) show that the integrated term in (5) is zero. There remains an integral which must vanish for all values of δq. This can be so only if the integrand is zero identically. Thus we have

$$\boxed{\frac{d}{dt}\,\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0}$$

When the system has more than one degree of freedom, the s different functions $q_i\,(t)$ must be varied independently in the principle of least action. We then obtain s equations of the form

$$\boxed{\frac{d}{dt}\,\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0} \qquad (i = 1, 2. \ldots s\ ) \tag{6}$$

These are the required differential equations , called in mechanics ***Lagrange's equations***. If the Lagrangian of a given mechanical system is known, the equations (6) give the relations between accelerations, velocities, and co-ordinates, i.e. they are equations of motion of the system.

Mathematically, the equations (6) constitute a set of s second-order equations for s unknown functions $q_i\,(t)$. The general solution contains $2s$ arbitrary constants. To determine these constants and thereby to define uniquely the motion of the system, it is necessary to know the initial conditions which specify the state of the

system at some given instant, for example the initial values of all the co-ordinates and velocities.

Note:

(i) The Lagrangian function of two weakly interacting systems A and B is given by the sum of the Lagrangian of the system A and B:

$L = L_A + L_B$

(ii) If two Lagrangian functions L' and L differ by a total time derivative of some function of co-ordinate and time i.e. if $L'(q, \dot{q}, t) = L(q, \dot{q}, t) + \frac{d}{dt} f(q, t)$,

then $S' = \int_{t_1}^{t_2} L'(q, \dot{q}, t)\, dt = \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt + \int_{t_1}^{t_2} \frac{d}{dt} f(q, t)\, dt$

or $S' = S + f\left(q^{(2)}, t_2\right) - f\left(q^{(1)}, t_1\right)$

i.e. S' differs from S by a quantity which gives zero on variation, so that the conditions $\delta S' = 0$ and $\delta S = 0$ are equivalent, and the form of the equations of motion unchanged. ***Thus the Lagrangian is defined only to within an additive total time derivative of any function of coordinate and time.***

1.4 Galileo's Relativity Principle

What is an inertial frame ?

"A frame of reference in which space is homogeneous and isotropic and time is homogeneous". In particular, in such a frame a free body which is at rest at some instant remains always at rest.

Largangian of a particle, moving freely, in an inertial frame of reference :

$$L = L(v^2) \qquad (1)$$

Since the Lagrangian is independent of $\vec{r}$, we have $\frac{\partial L}{\partial \vec{r}} = 0$, and so the Lagrange's equation's

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \vec{v}}\right) = 0$$

$$\therefore \frac{\partial L}{\partial \vec{v}} = constant$$

Since $\frac{\partial L}{\partial \vec{v}}$ is a function of the velocity only, it follows that $\vec{v} = constant$

Thus we conclude that, in an inertial frames, any free motion takes place with a velocity which is constant in both magnitude and direction. This the law of inertia".

If we consider, besides the inertial frame, another frame moving uniformly in a straight line relative to the inertial frame, then the lines of free motion in the other frame will be same as in original frame : Free motion takes place with a constant velocity.

Galileo's relativity principle :

"There is not a one but an infinity of inertial frames moving, relative to one another, uniformly in a straight line. In all these frames the properties of space and time are the same and the laws of mechanics are the same".

Galilean transformation :

$$\vec{r} = \vec{r'} + \vec{v}t \ , \ t = t'$$

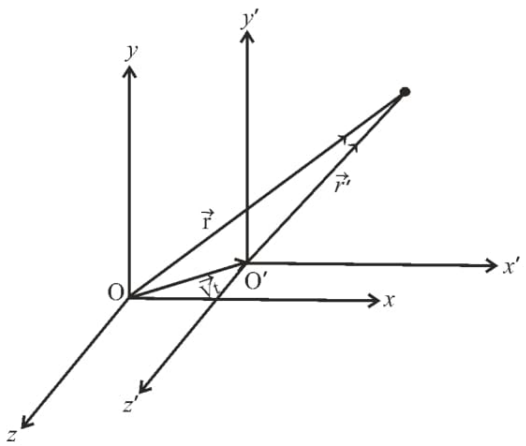


Figure 1.1

- **Lagrangian of a free particle :**

$$L = L\,(v^2)$$

In $x'y'z'$ frame velocity of the particle is $\vec{v'} = \vec{v} + \vec{\epsilon}$

$$\therefore L' = L\,(v'^2) = L\,(v^2 + 2\vec{v}.\vec{\epsilon} + \epsilon^2)$$

$$= L\,(v^2) + 2\vec{v}.\vec{\epsilon}\,\frac{\partial L}{\partial v^2}$$

Since the equations of motion in two inertial frames must be of same form

(Galileo's relativity principle). Then the two Lagrangians must differ only by a total time derivative of some function of $\vec{r}$ and t :

So the second term is a total time derivative as if $\frac{\partial L}{\partial v^2}$ is independent of velocity.

i.e. Lagrangian $\propto v^2$

and we write $L = \frac{1}{2}mv^2$

Example1.1 Show that Lagrangian $L = \frac{1}{2}mv^2$ satisfies Galileo's relativity principle

Sol. $\because L' = \frac{1}{2}mv'^2$

$$= \frac{1}{2}m(\vec{v} + \vec{V})^2$$

$$= \frac{1}{2}mv^2 + m\vec{v}.\vec{V} + \frac{1}{2}mV^2$$

$$= L + \frac{d}{dt}\left(m\vec{r}.\vec{V} + \frac{1}{2}mV^2t\right)$$

$$\therefore L' = L + total\ two\ derivative\ of\ some\ function$$

Action of a free particle S= $\int_1^2 \frac{1}{2}mv^2dt$

➢ Mass is positive and Lagrangian of a free particle in Cartesian, cylindrical and spherical polar coordinates.

(A) $L = \frac{1}{2}m\,(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$ (in Cartesian)

(B) $L = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\phi}^2 + \dot{z}^2\right)$ (in cylindrical)

(C) $L = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2 + \dot{r}^2 sin^2\theta\,\dot{\phi}^2\right)$(in spherical polar coordinate)

1.5 Self Learning Exercise

Q.1 Which of the following statements is true

(A)Lagrangian of a mechanical system is Unique

(B)Lagrangian is defined only to within an additive total time derivative of any function of coordinate and time.

(C)An inertial frame is unique

(D)Space-time properties differ in all inertial frames.

Q.2 The Lagrangian of a 'free' particle is

(A) $L \propto v$ (B) $L \propto v^2$

(C) $L \propto f(\vec{r})$ (D) $L \propto f(\vec{r},t)$

Q.3 What are generalized coordinates?

1.6 The Lagrangian for a System of Particles

Consider a system of particles which interact with one another but with no other bodies (closed system).

It is found that the interaction between the particles can be described by adding to the Lagrangian $\sum \frac{1}{2} m_a V_a^2$ a certain function of the coordinates, which depends on the nature of the interaction. Denoting this function by $-U$, we have

$$\boxed{L = T - U = \sum \frac{1}{2} m_a V_a^2 - U\left(\vec{r}_1, \vec{r}_2, \ldots\ldots\right)} \quad (1)$$

The sum $T = \sum \frac{1}{2} m_a V_a^2$ is K.E. of the system.

Knowing the Lagrangian, we can derive the equations of motion :

$$\frac{d}{dt} \frac{\partial L}{\partial \overrightarrow{V_a}} = -\frac{\partial V}{\partial \overrightarrow{r_a}} \quad (2)$$

Substitution of (1) gives

$$m_a \frac{d\overrightarrow{V_a}}{dt} = -\frac{\partial U}{\partial \overrightarrow{r_a}} \quad (3)$$

In this form the equations of motion are called Newton's equations and form the basis of mechanics of a system of interacting particles.

The vector $\vec{F} = -\frac{\partial U}{\partial \overrightarrow{r_a}}$ is called force on the a^{th} particle. U depends only on the a coordinates or particles and **Not** on their velocities.

The form of Lagrangian (1) shows that time is both homogeneous and isotropic, i.e. if $t \to -t$, Lagrangian is unchanged, and therefore so are the equation of motion.

In other words, if a given motion is possible in a system, then so is the reverse motion (that is, the motion in which the system passes through the same states in the reverse order). In this sense all motion which obey the laws of classical mechanics are reversible.The potential energy is defined only to within an additive constant which has no effect on the equation of motion.

If we use, to describe the motion, arbitrary generalized coordinates q_i instead of Cartesian coordinates, the following transformation is needed to obtain the new Lagrangian :

$$x_a = f_a(q_1, q_2, \dots \dots \dots q_s)$$

$$\dot{x}_a = \sum_k \frac{\partial f_a}{\partial q_k}\, \dot{q}_k \ , \ \ etc$$

Substituting these expressions in the function :

$$L = \frac{1}{2} \sum m_a \, (\dot{x}_a^2 + \dot{y}_a^2 + \dot{z}_a^2) - \ U$$

We obtain the required Lagrangian in the form

$$L = \frac{1}{2} \sum_{i,k} a_{i,k}(q) \dot{q}_i \dot{q}_k - \ U$$

Lagrangian of a system A which is not closed and interacts with another system B executing a given motion :

In such a case we say that the system A moves in a given external field (due to the system B).

The Lagrangian L_A of the system A can be found by using the Lagrangian L of the whole system A+B and replacing the coordinates q_B there in by given function of time.

Assuming that the system A+B is closed, we have

$$L = \ T_A(q_A \, , \dot{q}_A) + T(q_B, \dot{q}_B) - U(q_A \, , q_B)$$

Now omitting the term $T[q_B(t), \dot{q}_B \, (t)]$ which depends on time only and is therefore the total time derivative of a function of time we obtain :

$$L_A = T_A(q_A \, , \dot{q}_A) - U(q_A, q_B(t))$$

Thus the motion of a system in an external field is described by Lagrangian of the usual type, the only difference being that the potential energy may depend explicitly on time :

$$L = \frac{1}{2} \, mv^2 - U(\vec{r}, t)$$

$$m\dot{\vec{v}} = -\frac{\partial U}{\partial \vec{r_a}}$$

The P.E. of a uniform field is :

$$U = -\vec{F}.\vec{r}$$

➢ Atwood Machine

We consider the system as shown in the figure. Two bodies of mass m_1 and m_2 are connected by a string of length l that is suspended over a pulley. The string roll over the pulley without sliding. moment of inertia of the pulley is I. The Lagrange equation for the composite system can be obtained as

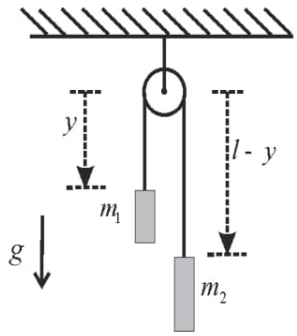


Figure 1.2

The radius of the pulley is R , the angular position ϕ

The potential energy of the system is

$$V = -m_1 gy - m_2 (d - y) g = (m_2 - m_1) gy - m_2 d$$

The kinetic energy $T = \frac{1}{2} m_1 \dot{y}^2 + \frac{1}{2} m_2 \dot{y}^2 + \frac{1}{2} I \dot{\phi}^2 = \frac{1}{2}\left(m_1 + m_2 + \frac{1}{R^2} \right) \dot{y}^2$

The Lagrangian

$$L = \frac{1}{2}\left(m_1 + m_2 + \frac{1}{R^2} \right) \dot{y}^2 + (m_1 - m_2) gy + m_2 d$$

Here we have $\frac{\partial L}{\partial y} = (m_1 - m_2) g$, $\frac{\partial L}{\partial \dot{y}} = \left(m_1 + m_2 + \frac{1}{R^2} \right) \dot{y}$

The Lagrange equation gives

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}} \right) - \frac{\partial L}{\partial y} = 0$$

$$\Rightarrow \left(m_1 + m_2 + \frac{I}{R^2} \right) \ddot{y} + (m_2 - m_1) g = 0$$

$$\Rightarrow \ddot{y} = \frac{m_1 - m_2}{m_1 + m_2 + \frac{I}{R^2}} g$$

This equation represents constant acceleration of the masses.

Pendulum with accelerated point of suspension

We take pendulum that performs oscillations in the $x, y - plane$, with y as the vertical direction. The mass of the pendulum bob is m and the pendulum rod has length l and is considered as massless and rigid. The suspension point moves s with constant acceleration in the $x-$ direction, so that

$x_A = \frac{1}{2}at^2,\ y_A = 0$ Here a as the (constant) acceleration

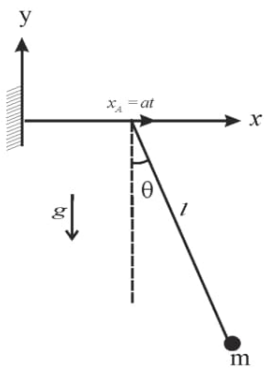


Figure 1.3

The pendulum moves in a plane .

The coordinates of the bob can be written as

$$x = x_A + l\sin\theta = l\sin\theta + \frac{1}{2}at^2$$

Thus $\dot{x} = l\dot{\theta}\cos\theta + at$

$$\dot{y} = l\dot{\theta}\sin\theta$$

The potential energy $V = -mgl\cos\theta$

and the kinetic energy

$$T = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right)$$

$$= \frac{1}{2}m\left(l^2\dot{\theta}^2 + 2atl\dot{\theta}\cos\theta + a^2t^2\right)$$

The Lagrangian

$$L=\frac{1}{2}m\left(l^2\dot{\theta}^2+2atl\dot{\theta}\cos\theta+a^2t^2\right)+mgl\cos\theta$$

Lagrange's equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}}\right)-\frac{\partial L}{\partial\theta}=0$$

Here $\dfrac{\partial L}{\partial\theta}=-matl\dot{\theta}\sin\theta-mgl\sin\theta$

$$\frac{\partial L}{\partial\dot{\theta}}=ml^2\dot{\theta}+matl\cos\theta$$

This gives $ml^2\ddot{\theta}+ml(g\sin\theta+\cos\theta)=0$

For convenience we introduce a fixed angle θ_0 defined by

$$g=\sqrt{g^2+a^2}\cos\theta_0,\ a=-\sqrt{g^2+a^2}\sin\theta_0$$

The equation of motion

$$ml^2\ddot{\theta}+ml\sqrt{g^2+a^2}\sin\left(\theta-\theta_0\right)=0$$

Example 1.2 For the elliptical wire, taking a and b to be constant, the Lagrangian is

$$L=T-U=\frac{m}{2}[a^2\dot{\alpha}^2\sin^2\alpha+b^2\dot{\alpha}^2\cos^2\alpha]-mgb\sin\alpha$$

Obtain the equation of motion.

Sol. $\dfrac{d}{dt}\left(\dfrac{\partial L}{\partial\dot{\alpha}}\right)=\dfrac{d}{dt}\left(\dfrac{\partial T}{\partial\dot{\alpha}}\right)$

$$=\frac{d}{dt}[m\dot{\alpha}\left(a^2\sin^2\alpha+b^2\cos^2\alpha\right)]$$

$$=m\ddot{\alpha}\left(a^2\sin^2\alpha+b^2\cos^2\alpha\right)+2m\dot{\alpha}^2\left(a^2-b^2\right)\sin\alpha\ \cos\alpha$$

$$\frac{\partial L}{\partial\alpha}=\frac{\partial T}{\partial\alpha}-\frac{\partial U}{\partial\alpha}$$

$$=2m\dot{\alpha}^2\left(a^2-b^2\right)\sin\alpha\cos\alpha-mgb\cos\alpha$$

The Lagrange equation is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\alpha}}\right)-\frac{\partial L}{\partial \dot{\alpha}}=0$$

$$m\ddot{\alpha}\left(a^2\sin^2\alpha+b^2\cos^2\alpha\right)+m\,gb\,\cos\alpha=0$$

Example 1.3 Point particle moves on the surface of a sphere. Obtain the equation of motion.

Sol. We consider a point particle of mass m that moves without friction on the surface of a sphere under the influence of gravitation. The gravitational field is assumed to point in the negative $z-$direction. This system has two degrees of freedom, since the three Cartesian coordinates (x,y,z) of the particle are subject to one constraint equation $r=\sqrt{x^2+y^2+z^2}=const.$ As generalized coordinates we chose the polar angles (ϕ,θ), so that the Cartesian coordinates are

$$x=r\cos\phi\sin\theta$$

$$y=r\sin\phi\sin\theta$$

$$z=r\cos\theta$$

with r as a constant. The corresponding velocities are

$$\dot{x}=r\left(\cos\phi\cos\theta\dot{\theta}-\sin\phi\sin\theta\dot{\phi}\right)$$

$$\dot{y}=r\left(\sin\phi\cos\theta\dot{\theta}+\cos\phi\sin\theta\dot{\phi}\right)$$

$$\dot{z}=-r\sin\theta\dot{\theta}$$

The potential energy is

$$V=mgz=mgr\cos\theta$$

with g as the acceleration of gravitation, and the kinetic energy is

$$T=\frac{1}{2}\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right)=\frac{1}{2}mr^2\left(\dot{\theta}^2+\sin^2\theta\dot{\phi}^2\right)$$

This gives the following expression for the Lagrangian

$$L=\frac{1}{2}mr^2\left(\dot{\theta}^2+\sin^2\theta\dot{\phi}^2\right)-mgr\cos\theta$$

Clearly ϕ *is a* ***cyclic coordinate,*** as $\dfrac{\partial L}{\partial \dot{\phi}}=0$

and therefore Lagrange's equation for this variable reduces to

$$\frac{\partial L}{\partial \dot{\phi}} = mr^2\dot{\phi}\sin^2\theta = l$$

with l as a constant. Lagrange's equation for the variable θ is

$$mr^2\ddot{\theta} - mr^2\dot{\phi}^2\sin\theta\cos\theta + mgr\sin\theta = 0$$

To eliminate the variable ϕ from the equation, we express, by use of (…), $\dot{\phi}$ in terms of the constant of motion l.

$$\dot{\phi} = \frac{l}{mr^2\sin^2\theta}$$

Inserted in (…) this gives

$$mr^2\ddot{\theta} - \frac{l^2\cos\theta}{mr^2\sin^3\theta} + mgr\sin\theta = 0$$

This illustrates the general discussion of cyclic coordinates. In the present case the elimination of the coordinate ϕ has reduced the equations of motion to one, and the only remaining trace of the coordinate ϕ is the appearance of the conserved quantity l in the equation.

Example 1.4 Find the Lagrangian and frequency of oscillations of the pendulum shown in the figure whose point of support carries a mass m_1 and is free to move horizontally on smooth wire along x axis. Masses m_1 and m_2 are connected by a light string of length *l*.

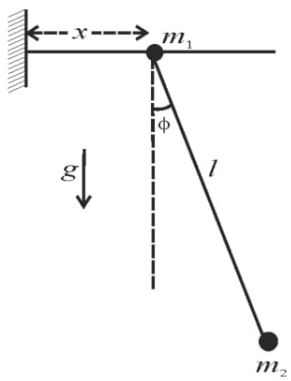


Figure 1.4

Sol. $x_2 = x_1 + l\sin\varphi, \quad \dot{x}_2 = \dot{x}_1 + l\cos\varphi\ \dot{\varphi}$

$y_2 = -l\cos\varphi, \quad \dot{y}_2 = l\sin\varphi\ \dot{\varphi}$

As gravity is in y direction and there is no force on the system of m_1 and m_2 along x direction. So x component of momentum P_X remains constant. The system is released from rest, so initial momentum of the system is zero.

$$P_x = m_1\dot{x}_1 + m_2\dot{x}_2 = 0$$

$$m_1\dot{x}_1 + m_2(\dot{x}_1 + l\cos\varphi\ \dot{\varphi}) = 0$$

$$\dot{x}_1 = -\frac{m_2 l\cos\varphi\ \dot{\varphi}}{(m_1 + m_2)}$$

Kinetic energy $T = T_1 + T_2 = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2(\dot{x}_2^2 + \dot{y}_2^2)$

$$= \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\left[\ \left(\dot{x}_1 + l\cos\varphi\dot{\varphi}\right)^2 + l^2\sin^2\varphi\dot{\varphi}^2\ \right]$$

$$= \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\left[\ \dot{x}_1^2 + l^2\cos^2\varphi\ \dot{\varphi}^2 + 2l\dot{x}_1\cos\varphi\dot{\varphi} + l^2\sin^2\varphi\dot{\varphi}^2\ \right]$$

$$T = \frac{1}{2}(m_1 + m_2)\dot{x}_1^2 + \frac{1}{2}m_2\left[l^2\dot{\varphi}^2 + 2l\dot{x}_1\cos\varphi\dot{\varphi}\right]$$

$$T = \frac{1}{2}(m_1 + m_2)\frac{m_2^2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)^2} + \frac{1}{2}m_2\left[l^2\dot{\varphi}^2 - \frac{2m_2 l\cos\varphi\dot{\varphi}}{(m_1 + m_2)}l\cos\varphi\dot{\varphi}\right]$$

$$= \frac{1}{2}\frac{m_2^2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)} + \frac{1}{2}m_2\left[l^2\dot{\varphi}^2 - \frac{2m_2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)}\right]$$

$$= \frac{1}{2}\frac{m_2^2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)} + \frac{1}{2}m_2 l^2\dot{\varphi}^2 - \frac{m_2^2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)}$$

$$= \frac{1}{2}m_2 l^2\dot{\varphi}^2 - \frac{1}{2}\frac{m_2^2 l^2\cos^2\varphi\dot{\varphi}^2}{(m_1 + m_2)}$$

$$= \frac{1}{2}m_2 l^2\dot{\varphi}^2\left[1 - \frac{m_2\cos^2\varphi}{(m_1 + m_2)}\right] = \frac{1}{2}m_2 l^2\dot{\varphi}^2\left[\frac{m_1 + m_2 - m_2\cos^2\varphi}{(m_1 + m_2)}\right]$$

$As\ \varphi << 1,\ \cos^2\varphi \to 1$ and $(m_2 - m_2\cos^2\varphi) \to 0$

$$T \cong \frac{1}{2}\frac{m_1 m_2}{(m_1 + m_2)}l^2\dot{\varphi}^2$$

Consider x axis as reference line for gravitational potential energy

$$U = m_1 g(0) + m_2 g(-l\cos\varphi) = -m_2 gl\cos\varphi$$

$$L = T - U = \frac{1}{2}\frac{m_1 m_2}{(m_1 + m_2)} l^2\dot{\varphi}^2 + m_2 gl\cos\varphi$$

Lagrangian equation of motion

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\varphi}} - \frac{\partial L}{\partial \varphi} = 0$$

$$\frac{d}{dt}\left(\frac{1}{2}\frac{m_1 m_2}{(m_1 + m_2)} 2l^2\dot{\varphi}\right) - m_2 gl(-\sin\varphi) = 0$$

$$\frac{m_1 m_2}{(m_1 + m_2)_2}\ l^2\ \ddot{\varphi} - m_2 gl(-\sin\varphi) = 0$$

$$\ddot{\varphi} + \frac{(m_1 + m_2)}{m_1}\frac{g}{l}\sin\varphi = 0$$

$$\ddot{\varphi} + \frac{(m_1 + m_2)}{m_1}\frac{g}{l}\varphi = 0 \quad (\because \text{For } \varphi << 1, \sin\varphi \cong \varphi)$$

$$\ddot{\varphi} + \omega^2\varphi = 0 \ \text{ where } \omega = \sqrt{\left(\frac{m_1 + m_2}{m_1}\right)\frac{g}{l}}$$

Example 1.5 Find the Lagrangian of the given double pendulum system when placed in a uniform gravitational field and determine the small oscillations of a coplanar double pendulum.

Sol. For convenience consider positive y direction in downward direction

$$x_1 = l_1\sin\varphi_1, y_1 = l_1\cos\varphi_1,$$

$$x_2 = x_1 + l_2\sin\varphi_2 = l_1\sin\varphi_1 + l_2\sin\varphi_2$$

$$y_2 = l_1\cos\varphi_1 + l_2\cos\varphi_2$$

$$\dot{x}_1 = l_1\cos\varphi_1\dot{\varphi}_1, \dot{y}_1 = -l_1\sin\varphi_1\dot{\varphi}_1,$$

$$\dot{x}_2 = l_1\cos\varphi_1\dot{\varphi}_1 + l_2\cos\varphi_2\dot{\varphi}_2$$

$$\dot{y}_2 = -l_1\sin\varphi_1\dot{\varphi}_1 - l_2\sin\varphi_2\dot{\varphi}_2$$

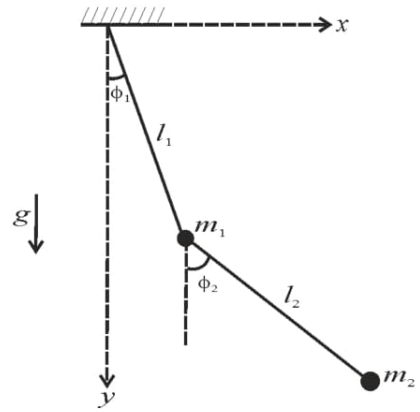


Figure 1.5

Kinetic energy of the system is

$$T = \frac{1}{2}m_1\left(\dot{x}_1^2 + \dot{y}_1^2\right) + \frac{1}{2}m_2\left(\dot{x}_2^2 + \dot{y}_2^2\right)$$

$$= \frac{1}{2}m_1 l_1^2\dot{\varphi}_1^2 + \frac{1}{2}m_2[\left(l_1^2\cos^2\varphi_1\dot{\varphi}_1^2 + l_2^2\cos^2\varphi_2\dot{\varphi}_2^2 + 2l_1\cos\varphi_1\dot{\varphi}_1 l_2\cos\varphi_2\dot{\varphi}_2\right)$$

$$+\left(l_1^2\sin^2\varphi_1\dot{\varphi}_1^2 + l_2^2\sin^2\varphi_2\dot{\varphi}_2^2 + 2l_1\sin\varphi_1\dot{\varphi}_1 l_2\sin\varphi_2\dot{\varphi}_2\right)]$$

$$= \frac{1}{2}m_1 l_1^2\dot{\varphi}_1^2 + \frac{1}{2}m_2[\left(l_1^2\dot{\varphi}_1^2 + l_2^2\dot{\varphi}_2^2 + 2l_1 l_2\dot{\varphi}_1\dot{\varphi}_2\{\cos\varphi_1\cos\varphi_2 + \sin\varphi_1\sin\varphi_2\}\right)]$$

$$= \frac{1}{2}(m_1 + m_2)l_1^2\dot{\varphi}_1^2 + \frac{1}{2}m_2 l_2^2\dot{\varphi}_2^2 + m_2 l_1 l_2\dot{\varphi}_1\dot{\varphi}_2\cos(\varphi_1 - \varphi_2)$$

Consider x axis as reference line for gravitational potential energy .Potential energy of the system is given by

$$\mathrm{U} = -m_1 g y_1 - m_2 g y_2 = -m_1 g l_1\cos\varphi_1 - m_2 g(l_1\cos\varphi_1 + l_2\cos\varphi_2)$$

$$= -(m_1 + m_2)g l_1\cos\varphi_1 - m_2 g l_2\cos\varphi_2$$

Lagrangian of the system is given by L = T-U

$$\mathrm{L} = \frac{1}{2}(m_1 + m_2)l_1^2\dot{\varphi}_1^2 + \frac{1}{2}m_2 l_2^2\dot{\varphi}_2^2 + m_2 l_1 l_2\dot{\varphi}_1\dot{\varphi}_2\cos(\varphi_1 - \varphi_2)$$

$$+(m_1 + m_2)g l_1\cos\varphi_1 + m_2 g l_2\cos\varphi_2$$

Lagrangian equation of motion

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{\varphi}_1} - \frac{\partial L}{\partial\varphi_1} = 0$$

$$\frac{d}{dt}\{(m_1+m_2)l_1^2\dot{\varphi}_1+m_2l_1l_2\dot{\varphi}_2\cos(\varphi_1-\varphi_2)\}+$$

$$m_2l_1l_2\dot{\varphi}_1\dot{\varphi}_2\sin(\varphi_1-\varphi_2)+(m_1+m_2)gl_1\sin\varphi_1=0$$

$$(m_1+m_2)l_1^2\ddot{\varphi}_1+m_2l_1l_2\ddot{\varphi}_2\cos(\varphi_1-\varphi_2)-m_2l_1l_2\dot{\varphi}_2(\dot{\varphi}_1-\dot{\varphi}_2)\sin(\varphi_1-\varphi_2)$$

$$+m_2l_1l_2\dot{\varphi}_1\dot{\varphi}_2\sin(\varphi_1-\varphi_2)+(m_1+m_2)gl_1\sin\varphi_1=0$$

$$\left(\frac{m_1}{m_2}+1\right)l_1^2\ddot{\varphi}_1+l_1l_2\ddot{\varphi}_2\cos(\varphi_1-\varphi_2)+l_1l_2\dot{\varphi}_2^2\sin(\varphi_1-\varphi_2)+\left(\frac{m_1}{m_2}+1\right)gl_1\sin\varphi_1=0 \quad (1)$$

Lagrangian equation of motion

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{\varphi}_2}-\frac{\partial L}{\partial\varphi_2}=0$$

$$\frac{d}{dt}\{m_2l_2^2\dot{\varphi}_2+m_2l_1l_2\dot{\varphi}_1\cos(\varphi_1-\varphi_2)\}$$

$$-m_2l_1l_2\dot{\varphi}_1\dot{\varphi}_2\sin(\varphi_1-\varphi_2)+m_2gl_2\sin\varphi_2=0$$

$$m_2l_2^2\ddot{\varphi}_2+m_2l_1l_2\ddot{\varphi}_1\cos(\varphi_1-\varphi_2)-m_2l_1l_2\dot{\varphi}_1(\dot{\varphi}_1-\dot{\varphi}_2)\sin(\varphi_1-\varphi_2)$$

$$-m_2l_1l_2\dot{\varphi}_1\dot{\varphi}_2\sin(\varphi_1-\varphi_2)+m_2gl_2\sin\varphi_2=0$$

$$l_2^2\ddot{\varphi}_2+l_1l_2\ddot{\varphi}_1\cos(\varphi_1-\varphi_2)-l_1l_2\dot{\varphi}_1^2\sin(\varphi_1-\varphi_2)+gl_2\sin\varphi_2=0 \quad (2)$$

For small oscillations $\phi_1 \ll 1,\ \ \phi_2 \ll 1$

$\sin\phi \approx \phi$ and $\cos\phi \approx 1$

From (1) and (2)

$$\left(\frac{m_1}{m_2}+1\right)l_1^2\ddot{\varphi}_1+l_1l_2\ddot{\varphi}_2+l_1l_2\dot{\varphi}_2^2(\varphi_1-\varphi_2)+\left(\frac{m_1}{m_2}+1\right)gl_1\varphi_1=0 \quad (2a)$$

$$l_2^2\ddot{\varphi}_2+l_1l_2\ddot{\varphi}_1-l_1l_2\dot{\varphi}_1^2(\varphi_1-\varphi_2)+gl_2\varphi_2=0 \quad (2b)$$

Neglecting the terms $\dot{\phi}_2^2$ and $\dot{\phi}_1^2$ in eq.(2a) and (2b),we have

$$\left(\frac{m_1}{m_2}+1\right)l_1\ddot{\varphi}_1+l_2\ddot{\varphi}_2+\left(\frac{m_1}{m_2}+1\right)g\varphi_1=0 \quad (3)$$

$$l_2\ddot{\varphi}_2+l_1\ddot{\varphi}_1+g\varphi_2=0 \quad (4)$$

Let$\phi_k = A_k e^{i\omega t}$ $i.e.\ \phi_1 = A_1 e^{i\omega t}$, $\phi_2 = A_2 e^{i\omega t}$

Putting these quantities in eq (3) and (4)

$$\left(\frac{m_1}{m_2}+1\right) l_1 A_1 (i\omega)^2 e^{i\omega t} + l_2 A_2 (i\omega)^2 e^{i\omega t} + \left(\frac{m_1}{m_2}+1\right) g A_1 e^{i\omega t} = 0$$

$$-\left(\frac{m_1}{m_2}+1\right) l_1 A_1 \omega^2 - l_2 A_2 \omega^2 + \left(\frac{m_1}{m_2}+1\right) g A_1 = 0$$

$$\left(\frac{m_1}{m_2}+1\right)\left(g - l_1 \omega^2\right) A_1 - l_2 \omega^2 A_2 = 0 \qquad (5)$$

From (4)

$$l_2 A_2 (i\omega)^2 e^{i\omega t} + l_1 A_1 (i\omega)^2 e^{i\omega t} + g_2 A_2 e^{i\omega t} = 0$$

$$l_2 A_2 \omega^2 + l_1 A_1 \omega^2 - g A_2 = 0$$

$$A_1 l_1 \omega^2 + \left(l_2 \omega^2 - g\right) A_2 = 0 \qquad (6)$$

From (5) and (6),for roots of characteristic equation

$$\begin{vmatrix} \left(\frac{m_1}{m_2}+1\right)\left(g - l_1 \omega^2\right) & -l_2 \omega^2 \\ l_1 \omega^2 & \left(l_2 \omega^2 - g\right) \end{vmatrix} = 0$$

$$\left(\frac{m_1}{m_2}+1\right)\left(\omega^2 g l_2 - g^2 - \omega^4 l_1 l_2 + \omega^2 g l_1\right) + \omega^4 l_1 l_2 = 0$$

$$\omega^4 l_1 l_2 \left[1 - \left(\frac{m_1}{m_2}+1\right)\right] + \omega^2 g (l_1 + l_2)\left(\frac{m_1}{m_2}+1\right) - g^2\left(\frac{m_1}{m_2}+1\right) = 0$$

$$\omega^4 l_1 l_2 m_1 - \omega^2 g (l_1 + l_2)(m_1 + m_2) + g^2 (m_1 + m_2) = 0$$

$$\omega^2 = \frac{g}{2 m_1 l_1 l_2}\left[(l_1 + l_2)(m_1 + m_2) \pm \sqrt{(m_1 + m_2)}\sqrt{(m_1 + m_2)(l_1 + l_2)^2 - 4 m_1 l_1 l_2}\right]$$

$$\omega^2 = \frac{g}{2 l_1 l_2}\left[(l_1 + l_2)\left(1 + \frac{m_2}{m_1}\right) \pm \sqrt{\left(1 + \frac{m_2}{m_1}\right)}\sqrt{\left(1 + \frac{m_2}{m_1}\right)(l_1 + l_2)^2 - 4 l_1 l_2}\right]$$

$$If\ m_1 \to \infty\ \ then \left(1+\frac{m_2}{m_1}\right) \to 1 \text{ and}$$

$$\omega^2 \approx \frac{g}{2l_1 l_2}\left[(l_1+l_2) \pm \sqrt{(l_1+l_2)^2 - 4l_1 l_2}\right]$$

$$\omega^2 \approx \frac{g}{2l_1 l_2}\left[(l_1+l_2) \pm (l_1-l_2)\right]$$

$the\ frequencies\ tend\ to \sqrt{\frac{g}{l_1}}\ and \sqrt{\frac{g}{l_2}}$ corresponding to independent oscillations of the two pendulums.

1.7 Summary

We have derived the Lagrange's equations form the most fundamental law governing the motion of mechanical system viz. principle of least action or Hamilton's principle. According to which every mechanical system is characterized by a definite function $L(q,\dot{q},t)$. The function L is called the Lagrangian of the system and it satisfies a second-order differential equation viz- Lagrange's equations. From the very general properties of space and time in an inertial frame, we have derived the Galileo's relativity principle we have found the Lagrangian for a system of particles.

1.8 Glossary

Relativity **:**the state of being judged in comparison with other things and not by itself

Degrees of Freedom : number of independent coordinates to describe a system

1.9 Answers to Self Learning Exercise

Ans.1: B **Ans.2:** B

1.10 Exercise

Q.1 The Lagrangian of a system in an external field is

(A) $L=\frac{1}{2}mv^2$ (B) $L=\frac{1}{2}mv^2 - U(\vec{r})$

(C) $L=\frac{1}{2}mv^2-U(\vec{r},t)$ (D) $L=T+U$

Q.2 The Lagrangian of a particle in terms of the generalized coordinates is

(A) $\frac{1}{2}\sum_{i,k}a_{ik}(q)\dot{q}_i\dot{q}_k-U$ (B) $\frac{1}{2}\sum_{i}a_i(q)\dot{q}_i^2-U$

(C) $\frac{1}{2}\sum_{i,k}a_{ik}(q)q_i q_k-U$ (D) $\frac{1}{2}\sum_{i,k}a_{ik}(\dot{q})\dot{q}_i\dot{q}_k-U$

Q.3 Lagrangian of a free particle in cylindrical coordinates is

(A) $L=\frac{1}{2}m\left(\dot{r}^2+r^2\dot{\phi}^2+\dot{z}^2\right)$ (B) $L=\frac{1}{2}m\left(\dot{r}^2+\dot{\phi}^2+\dot{z}^2\right)$

(C) $L=\frac{1}{2}m\left(\dot{r}^2+\dot{r}^2\dot{\phi}^2+\dot{z}^2\right)$ (D) $L=\frac{1}{2}m\left(\dot{r}^2+r^2\sin\phi\,\dot{\phi}^2+\dot{z}^2\right)$

Q.4 Pendulum bob of radius R (where R>*r*).Construct the Lagrangian.

Q.5 Find the equation of motion of one dimensional harmonic oscillator using Hamilton's principle.

Q.6 A bead slides on a wire in the shape of the cycloid that described by equations

$x=a(\theta-\sin\theta)$

$y=a(1+\cos\theta)$ $\quad where\, 0\le\theta\le 2\pi$

Find(i)Lagrangian(ii)equation of motion

Here friction between bead and wire is negligible.

Q.7 Obtain the Lagrangian and equations of motion for the double pendulum. Here the lengths of pendula are l_1 and l_2 with corresponding to masses m_1 and m_2.

1.11 Answers to Exercise

Ans.1: C **Ans.2:** A

Ans.3: A

Ans.6: (i) $L=ma^2\dot{\theta}^2(1-\cos\theta)-mga(1+\cos\theta)$

(ii) $\ddot{\theta}(1-\cos\theta)+\frac{1}{2}\sin\theta\dot{\theta}^2-\frac{g}{2a}\sin\theta=0$

References and Suggested Readings

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UNIT-2
Conservation Laws

Structure of the Unit

2.0 Objectives

2.1 Introduction

2.2 Conservation Laws

2.3 Center of Mass

2.4 Self Learning Exercise

2.5 Angular Momentum

2.6 Summary

2.7 Glossary

2.8 Answer to Self Learning Exercise

2.9 Exercise

2.10 Answers to Exercise

References and Suggested Readings

2.0 Objectives

In this chapter we shall focus upon the homogeneity of system and conservation laws. Specifically we shall focus upon the following topics :

- Homogeneity of Time and Conservation Law of Energy
- law of conservation of momentum
- law of conservation of angular momentum.
- Relation between Mechanical energy of the system in Center of mass and Laboratory frames
- Angular momentum of the system in K and K' frames

2.1 Introduction

In this chapter we will study the close relationship between the symmetries

of space and time with respect to an inertial frame and conservation laws. ***The Lagargian of a closed system remains unaffected by an infinitesimal rotation of the system because the space is isotropic. This will lead to "law of conservation of angular momentum". Similarly homogeneity of space will lead to law of conservation of momentum. Law of conservation of energy follows from the "homogeneity of time"*** i.e. all instants of time are equivalent in an inertial frame. We shall study these laws of nature in this chapter

2.2 Conservation Laws

Integrals of Motion:

A. What are "Integrals of Motion" ?

During the motion of a mechanical system, the '*2s*' quantities q_i and $\dot{q}_i$ (i = 1, 2, ... *s*) which specify the state of the system vary with time. There exist, however, functions of these quantities whose values remain constant during the motion, and depend only on the initial conditions. Such functions are called "integrals of motion".

B. Show that the number of independent integrals of the motion for a closed mechanical system with '*s*' degrees of freedom is (2*s* –1).

As we know that Lagrange's equations $\frac{d}{dt}\frac{\partial L}{\partial q_i} - \frac{\partial L}{\partial \dot{q}_i} = 0$ constitute a set of '*s*' second – order equations for '*s*' unknown function $q_i(t)$. So, the general solution contains '*2s*'arbitrary constants. To determine these constants and thereby to define uniquely the motion of the system, it is necessary to know the initial conditions which specify the state of the system at some given instant, for example the initial values of all the coordinates q_i and velocities $\dot{q}_i$.

We shall show that the number of independent integrals of the motion for a closed mechanical system with '*s*' degrees of freedom is (2*s* –1).

This is evident from the following simple arguments. The general solutions of the equations of motion contains *2s* arbitrary constants. Since the equations of motion for a closed system do not involve the time explicitly, the choice of the origin of time is entirely arbitrary, and one of the arbitrary constants in the solution of the equations can always be taken as an additive constant t_0 in the time.

Eliminating $t+t_0$ from the *2s* functions

$q_i = q_i(t+t_0, c_1, c_2, ..., c_{2s-1})$

$\dot{q}_i = \dot{q}_i(t+t_0, c_1, c_2, ..., c_{2s-1})$,We can express the $(2s-1)$ (arbitrary constant $c_1, c_2, ...c_{2s-1}$ as functions of q and $\dot{q}$ and these functions will be integrals of the motion.

C. What are additive Integrals of Motion?

Not-all integrals of the motion are of equal importance in mechanics. There are some whose constancy is of profound significance, deriving from the fundamental homogeneity and isotropy of space and time. The quantities represented by such integrals of the motion are said to be conserved and have an important common property of being additive. Their values for a system composed of several parts whose interaction is negligible are equal to the sum of their values for the individual parts. It is to this additivity that the quantities concerned over their special importance in mechanics.

let us suppose, for example, that two bodies interact during a certain interval of time. Since each of the additive integrals of the whole system is, both before and after the interaction, equal to the sum of its values for the two bodies separately, the conservation laws for these additive quantities immediately make possible various conclusions regarding the state of the bodies after the interaction.

Homogeneity of Time and Conservation Law of Energy:

Derivation of the law of conservation of energy from the principle of "homogeneity of time:

By the homogeneity of time we mean that all instants of time are equivalent in an inertial frame. Because of this homogeneity, the Lagrangian $L(q_i, \dot{q}_i)$ of allowed system does not depend explicitly on time.

The total time derivative of the Lagrangian can therefore be written

$$\frac{dL}{dt} = \sum_i \frac{\partial L}{\partial q_i}\ \dot{q}_i + \sum_i \frac{\partial L}{\partial \dot{q}_i}\ \ddot{q}_i \qquad (2.1)$$

Note that we have omitted the term $\frac{\partial L}{\partial t}$ in this time derivative. The reason being that Lagrangian does not depend explicitly on time.

$$\because \boxed{p_i = \frac{\partial L}{\partial \dot{q}_i}, \dot{p}_i = \frac{\partial L}{\partial q_i}} \Rightarrow \dot{p}_i = \frac{dp_i}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial q_i}\right)$$

$$\dot{p} = \frac{\partial L}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial L}{\partial q_i}\right)$$

Replacing $\frac{\partial L}{\partial q_i}$ by $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)$ according to Lagrange's equation. From eq.(2.1) we get,

$$\frac{dL}{dt} = \sum_i \dot{q}_i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) + \sum_i \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i$$

$$= \sum_i \left(\dot{q}_i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i\right)$$

$$= \frac{d}{dt}\sum_i \left(\dot{q}_i \frac{\partial L}{\partial \dot{q}_i}\right)$$

or $$\frac{d}{dt}\left(\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L\right) = 0$$

Hence we see that the quantity

$$\boxed{E = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L} \qquad (2.2)$$

remains constant during the motion of closed system.

i.e. ***it is an integral of the motion, it is called the "energy" of the system***.

The additivity of E follows from that of Lagrangian, since Eq. (2.2) shows that it is a linear function of the Lagrangian.

Important Note:

1. The law of conservation of energy is valid not only for closed systems, but also for those in a constant external field (i.e. one independent of time). The only property of the Lagrangian used in the above derivation, namely that it does not involve the time explicitly, is still valid. Mechanical system whose energy is conserved are sometime called "conservative" systems.

2. As we know that the K.E. of a system of particles in terms of generalized

coordinates is given by $\boxed{T = \sum_{i,k} a_{ik}(q)\, \dot{q}_i\, \dot{q}_k}$ i.e. Kinetic Energy T is a quadratic function of velocities and one can express $T = T(q, \dot{q})$

$\therefore$ $\boxed{L = T(q,\dot{q}) - U(q)}$, where T is quadratic function of velocity.

Using Euler's theorem on homogeneous functions, we have

$$\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} = \sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2T$$

Therefore by eq.(2.2)

$$E = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L$$

$$= 2T - (T - U) \quad = T + U$$

Or $E = T(q,\dot{q}) + U(q)$

In Cartesian coordinates

$$E = \sum_a \frac{1}{2} m_a v_a^2 + U(\vec{r}_1, \vec{r}_2, \ldots) \qquad (2.3)$$

Thus the energy of the system can be written as the sum of two quite different terms: the kinetic energy, which depends on the velocities, and the potential energy, which depends only on the coordinates of the particles.

Homogeneity of Space and Law of Conservation of Momentum:

A second conservation law follows from the 'homogeneity of space'. This means that the mechanical properties of a closed system are unchanged by any parallel displacement of the entire system in space.

A parallel displacement is a transformation in which every particle in the system is moved by the same amount, the radius vector $\vec{r}$ becomes $\vec{r} + \vec{\varepsilon}$, where $\vec{\varepsilon}$ is infinitesimal displacement. Under this displacement, the Lagrangian remains unchanged.

The change in L resulting from an infinitesimal change in coordinates, the velocities of the particles remaining fixed, is

$$\delta L = \sum_a \frac{\partial L}{\partial \vec{r}_a} . \delta \vec{r}_a = \vec{\varepsilon} . \sum_a \frac{\partial L}{\partial \vec{r}_a}$$

The condition that $\delta L = 0$ implies $\sum_a \frac{\partial L}{\partial \vec{r}_a} = 0$

From Lagrange's equations we therefore have

$$\frac{d}{dt}\sum_a \frac{\partial L}{\partial \vec{v}_a} = 0$$

$$\therefore \sum_a \frac{\partial L}{\partial \vec{v}_a} = \text{Constant}$$

$$\text{or } \vec{P} = \text{Constant} \qquad \left(\text{where } \vec{P} = \sum_a \frac{\partial L}{\partial \vec{v}_a}\right)\left\{\because\ p_i = \frac{\partial L}{\partial \dot{q}_i}\right\}$$

$$\text{or } \sum_a m_a \vec{v}_a = \text{Constant}.$$

The additivity of the momentum is evident. Moreover, unlike the energy, the momentum of the system is equal to the sum of its values $\vec{p}_a = m_a \vec{v}_a$ for the individual particles, whether or not the interaction between them can be neglected.

Note:-

- The three components of the momentum vector are conserved only in the absence of an external field.
- The individual components may be conserved even in the presence of the a field ,however ,if the potential energy in the field does not depend on all the Cartesian coordinates ,the mechanical properties of the system are evidently unchanged by displacement along the axis of a coordinate which does not appear in the potential energy .For example ,in a uniform field in the z direction ,the x and y components of the momentum are conserved.
- $\because \frac{\partial L}{\partial \vec{r}_a} = -\frac{\partial U}{\partial r_a}$

Therefore the equation $\sum_a \frac{\partial L}{\partial \vec{r}_a} = 0$ implies $\sum_a \vec{F}_a = 0$ i.e. the sum of the forces on all the particles in a system is zero.

- $p_i = \frac{\partial L}{\partial \dot{q}_i}$ are called ***generalized momenta***.

$F_i = \dfrac{\partial L}{\partial q_i}$ are called ***generalized forces.***

In this notation Lagrangian equations are $\dot{p}_i = F_i$

2.3 Center of Mass

Frame K' moves relative to frame K with velocity $\vec{V}$. Let $\vec{v}_a$ be velocity of particle with respect to frame K and $\vec{v}'_a$ be velocity of particle with respect to frame K'

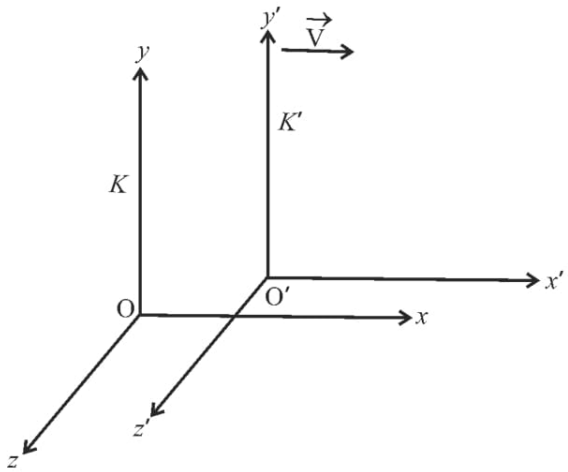


Figure 2.1

$$\therefore \qquad \vec{v}_a = \vec{v}'_a + \vec{V} \tag{2.4}$$

The momenta $\vec{P}$ and $\vec{P}'$ in two frames are therefore related by

Let $\vec{P} = \sum_a m_a \vec{v}_a$ (2.5)

be momentum of system of the particles with respect to frame K

Here particle of mass m_a has velocity $\vec{v}_a$.

Let $\vec{P}' = \sum_a m_a \vec{v}'_a$ (2.6)

be momentum of system of the particles with respect to frame K'

$$\therefore \vec{P} = \sum_a m_a \vec{v}_a = \sum_a m_a \left(\vec{v}'_a + \vec{v}\right) = \sum_a m_a \vec{v}'_a + \sum_a m_a \vec{v}$$

$$\boxed{\vec{P} = \vec{P}' + \vec{V}\sum_a m_a} \tag{2.7}$$

In particular, there is always a frame of reference in which the total momentum $\vec{P}'$ is zero. Putting $\vec{P}' = 0$ in eq.(2.7) ,we find the velocity of this particular frame

$$\vec{P} = 0 + \vec{V}\sum_a m_a$$

$$\Rightarrow \boxed{\vec{V} = \frac{\vec{P}}{\sum_a m_a} = \frac{\sum_a m_a \vec{v}_a}{\sum_a m_a}} \tag{2.8}$$

$$\frac{d\vec{R}}{dt} = \frac{\sum_a m_a \frac{d\vec{r}_a}{dt}}{\sum_a m_a}$$

$$\frac{d\vec{R}}{dt} = \frac{d}{dt}\left(\frac{\sum_a m_a \vec{r}_a}{\sum_a m_a}\right)$$

$\therefore$ $\boxed{\vec{R} = \frac{\sum_a m_a \vec{r}_a}{\sum_a m_a}}$ is a called position vector of Centre of Mass(C.M.) (2.9)

- In considering the mechanical properties of a closed system it is natural to use a frame of reference in which the center of mass is at rest. This eliminates a uniform rectilinear motion of the system as a whole, but such motions is of no interest.

- The energy of a mechanical system which is at rest as a whole(i.e. CM at rest) is usually called its "internal energy" E_i. This includes the kinetic energy of relative motion of the particles in that system and the potential energy of their interaction. The total energy of a system moving as a whole with velocity V can be written as $\boxed{E = \frac{1}{2}\mu V^2 + E_i}$ (2.10)

Where $\mu = \sum_a m_a$ is the total mass of the system (2.11)

- This formula can be proved easily. The relation between energies E and E' of a mechanical system in two frames K and K' are related by:

$$E = \sum_a \frac{1}{2} m_a v_a^2 + U$$

Where U is the potential energy of the system.

$$E = \frac{1}{2} \sum_a m_a v_a^2 + U$$

By eq.(2.4)

$$E = \frac{1}{2} \sum_a m_a \left(\vec{v}_a' + \vec{V} \right)^2 + U$$

$$= \frac{1}{2} \sum_a \left(m_a v_a'^2 + m_a V^2 + m_a 2\vec{v}_a' . \vec{V} \right) + U$$

$$= \frac{1}{2} \sum_a m_a v_a'^2 + \frac{1}{2} \sum_a m_a V^2 + \sum_a m_a \vec{v}_a' . \vec{V} + U$$

$$= \frac{1}{2} \sum_a m_a v_a'^2 + \frac{1}{2} V^2 \sum_a m_a + \vec{V} . \sum_a m_a \vec{v}_a' + U$$

$$= \frac{1}{2} \mu V^2 + \vec{V} . \sum_a m_a \vec{v}_a' + E'$$

$$E = \frac{1}{2} \mu V^2 + \vec{V} . \vec{P}' + E' \qquad (2.12)$$

Where $\vec{P}' = \sum_a m_a \vec{v}_a'$ and $E' = \frac{1}{2} \sum_a m_a v_a'^2 + U$ is the total energy of the system with respect to frame K'

If K' is the center of mass frame then in that frame.

$\vec{P}' = \vec{0}$, then E' is known as internal energy E_i

By eq(2.12)

$$E = \frac{1}{2} \mu V^2 + 0 + E'$$

$$\therefore E = E_i + \frac{1}{2} \mu V^2$$

Example 2.1 Find the law of transformation of the action $S = \int L(q, \dot{q}, t)dt$ from one inertial frame to another where L is the Lagrangian of the system .

Sol. We can follow the procedure similar to the Law of transformation of energy, we can write

$$L = T - U$$

$$\Rightarrow L = \sum_a \frac{1}{2} m_a v_a^2 - U$$

Using eq.(2.4)

$$L = \frac{1}{2}\sum_a m_a \left(\vec{v}_a' + \vec{V}\right)^2 - U$$

$$= \frac{1}{2}\sum_a \left(m_a v_a'^2 + m_a V^2 + m_a 2\vec{v}_a'.\vec{V}\right) - U$$

$$= \frac{1}{2}\sum_a m_a v_a'^2 + \frac{1}{2}\sum_a m_a V^2 + \sum_a m_a \vec{v}_a'.\vec{V} - U$$

$$= \frac{1}{2}\sum_a m_a v_a'^2 + \frac{1}{2}V^2 \sum_a m_a + \vec{V}.\sum_a m_a \vec{v}_a' - U$$

$$= \frac{1}{2}\mu V^2 + \vec{V}.\sum_a m_a \vec{v}_a' + \frac{1}{2}\sum_a m_a v_a'^2 - U$$

$$L = \frac{1}{2}\mu V^2 + \vec{V}.\vec{P}' + L' \qquad (2.13)$$

Where $\vec{P}' = \sum_a m_a \vec{v}_a'$ and $L' = \frac{1}{2}\sum_a m_a v_a'^2 + U$ is the total energy of the system with

Integrating the eq.(2.13)

$$\int L dt = \int \frac{1}{2}\mu V^2 dt + \int \vec{V}.\vec{P}' dt + \int L' dt$$

$$S = \int \frac{1}{2}\mu V^2 dt + \int \vec{V}.\vec{P}' dt + S'$$

$$S = \frac{1}{2}\mu V^2 \int dt + \vec{V}.\int \vec{P}' dt + S' \qquad (2.14)$$

$$\because \vec{P}' = \sum_a m_a \vec{v}'_a = \sum_a m_a \frac{d\vec{r}'_a}{dt} = \frac{d}{dt}\sum_a m_a \vec{r}'_a$$

$$= \sum_a m_a \frac{d}{dt}\left(\frac{\sum_a m_a \vec{r}'_a}{\sum_a m_a}\right) = \mu \frac{d}{dt}\left(\frac{\sum_a m_a \vec{r}'_a}{\sum_a m_a}\right) = \mu \frac{d\vec{R}'_{CM}}{dt}$$

Where $\vec{R}'_{CM}$ is the radius vector of the center of mass in the frame K'.

Putting this value of $\vec{P}'$ in the eq.(2.14)

$$S = \frac{1}{2}\mu V^2 \int dt + \mu \vec{V}.\int \frac{d\vec{R}'_{CM}}{dt} dt + S'$$

$$S = S' + \mu \vec{V}.\vec{R}'_{CM} + \frac{1}{2}\mu V^2 t$$

Example 2.2 A particle of mass m moves inside a bowl. If the surface of the bowl is given by the equation $z = \frac{1}{2}a\left(x^2 + y^2\right)$, where a is a constant, the Lagrangian of the particle is

1. $\frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\phi}^2 - gar^2\right)$
2. $\frac{1}{2}m\left[\left(1 + a^2r^2\right)\dot{r}^2 + r^2\dot{\phi}^2\right]$
3. $\frac{1}{2}m\left[\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\ \dot{\phi}^2 - gar^2\right]$
4. $\frac{1}{2}m\left[\left(1 + a^2r^2\right)\dot{r}^2 + r^2\dot{\phi}^2 - gar^2\right]$

Sol. Taking z=0 as reference level for gravitational potential energy.

$$U = mgz = mg\frac{a}{2}\left(x^2 + y^2\right) = \frac{1}{2}mgar^2$$

$\because$ In cylindrical coordinates $r^2 = x^2 + y^2$

$$\boxed{K.E. = T = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\varphi}^2 + \dot{z}^2\right)}$$

Here $z = \frac{a}{2}\left(x^2 + y^2\right) = \frac{1}{2}ar^2$

$$\Rightarrow \dot{z} = \frac{1}{2} 2ar\dot{r} = ar\dot{r}$$

$$\Rightarrow T = \frac{1}{2} m\left(\dot{r}^2 + r^2\dot{\varphi}^2 + a^2r^2\dot{r}^2\right)$$

$$= \frac{1}{2} m\left[\dot{r}^2(1 + a^2r^2) + r^2\dot{\varphi}^2\right]$$

$$\Rightarrow L = T - U = \frac{1}{2} m\left[\dot{r}^2(1 + a^2r^2) + r^2\dot{\phi}^2\right] - \frac{1}{2} mgar^2$$

$$L = \frac{1}{2} m[\dot{r}^2(1 + a^2r^2) + r^2\dot{\phi}^2 - gar^2]$$

Example 2.3 A Particle of mass m moving with velocity $\vec{v}_1$ leaves a half-space in which its potential energy is a constant U_1 and enters another region in which its P.E. is a different constant U_2. Determine the change in the direction of motions of the particle.

Sol. Let z=0 plane separates the both potential regions, therefore component of velocity of the particle in z plane remains constant .

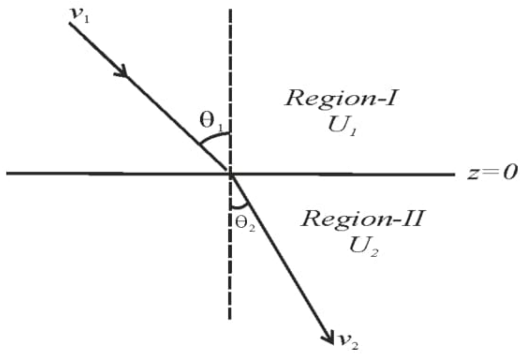


Figure 2.2

Following the boundary condition $[v_z]_I = [v_z]_{II}$

or $v_1 \sin\theta_1 = v_2 \sin\theta_2$ (boundary condition)

Energy conservation gives

$$\frac{1}{2} mv_1^2 + U_1 = \frac{1}{2} mv_2^2 + U_2$$

$$\Rightarrow \frac{1}{2} m\left[v_1^2 - v_2^2\right] = U_2 - U_1$$

$$\Rightarrow \; v_1^2 - v_2^2 = \frac{2}{m}(U_2 - U_1)$$

$$\Rightarrow v_1^2 - v_1^2 \frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{2}{mv_1^2}(U_2 - U_1)$$

$$\Rightarrow 1 - \frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{2}{v_1^2 m}(U_2 - U_1)$$

$$\Rightarrow \frac{\sin^2\theta_1}{\sin^2\theta_2} = 1 - \frac{2}{mv_1^2}(U_2 - U_1)$$

$$\Rightarrow \frac{\sin\theta_1}{\sin\theta_2} = \sqrt{1 - \frac{2}{v_1^2 m}(U_2 - U_1)}$$

$$\Rightarrow \frac{\sin\theta_1}{\sin\theta_2} = \sqrt{1 + \frac{2}{mv_1^2}(U_1 - U_2)}$$

2.4 Self Learning Exercise

Q.1 How do the energies E and E' in two inertial frames K and K' are related? K'-frame is moving with velocity V with respect to K-frame.

(A) $E = E' + \frac{1}{2}\mu V^2$ (B) $E = \frac{1}{2}\mu V^2 + \vec{V}.\vec{P}'$

(C) $E = E' + \frac{1}{2}\mu V^2 + \vec{V}.\vec{P}'$ (D) $E = E'$

Q.2 What do you mean by homogeneity of time and conservation law of energy.

2.5 Angular Momentum

Let us now derive the conservation law which follows from the ***isotropy of space.*** This isotropy means that the mechanical properties of a closed system do not vary which it is rotated as a whole in any manner in space.

- We therefore consider an infinitesimal rotation of the system, and obtain the condition for the Lagrangian to remain unchanged.

We make use of the vector $\delta\vec{Q}$ of the infinitesimal rotation, whose magnitude is angle of rotation δQ, and whose direction is that of the axis of rotation (the direction of rotation being that of a right-handed screw driven along $\delta\vec{Q}$).

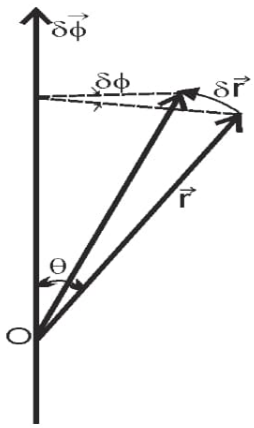


Figure 2.3

From the diagram it is clear that

$$\overrightarrow{OA} = \vec{r},\ CA = r\sin\theta\ ,\ \delta Q = \frac{AB}{CA} = \frac{|\delta\vec{r}|}{r\sin\theta}$$

$$|\delta\vec{r}| = r\sin\theta\,\delta Q$$

$$\delta\vec{r} = \delta\vec{Q}\times\vec{r} \qquad (2.15)$$

- When the system is rotated, and only the radius vectors but also the velocities of the particles change direction, and all values are transformed in the same manner. In similar way to eq.(1)the velocity increment relative to a fixed system of co-ordinates is

$$\delta\vec{v} = \delta\vec{Q}\times\vec{v} \qquad (2.16)$$

$$\because \quad \delta L = \sum_a \left\{ \frac{\partial L}{\partial \vec{r}_a}.\delta\vec{r}_a + \frac{\partial L}{\partial \vec{v}_a}.\delta\vec{v}_a \right\} = 0$$

$$\Rightarrow \sum_a \left\{ \dot{\vec{p}}_a.\delta\vec{r}_a + \vec{p}_a.\delta\vec{v}_a \right\} = 0 \qquad \left\{ \because\ \dot{p}_i = \frac{\partial L}{\partial q_i}\ ,\ p = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial v_i} \right\}$$

By eq.(2.15) &(2.16)

$$\Rightarrow \sum_a \left\{ \dot{\vec{p}}_a.\left(\delta\vec{Q}\times\vec{r}_a\right) + \vec{p}_a.\left(\delta\vec{Q}\times\vec{v}_a\right) \right\} = 0$$

$$\Rightarrow \delta\vec{Q}.\sum_a \left(\vec{r}_a\times\dot{\vec{p}}_a + \vec{v}_a\times\vec{p}_a \right) = 0 \qquad \left\{ \because\ \vec{A}.\left(\vec{B}\times\vec{C}\right) = \vec{B}.\left(\vec{C}\times\vec{A}\right) \right\}$$

$$\Rightarrow \delta\vec{Q}.\sum_a \left(\vec{r}_a\times\frac{d\vec{p}_a}{dt} + \frac{d\vec{r}_a}{dt}\times\vec{p}_a \right) = 0$$

$$\Rightarrow \delta\vec{Q}.\sum_a \frac{d}{dt}(\vec{r}_a \times \vec{p}_a) = 0$$

$$\Rightarrow \delta\vec{Q}.\frac{d}{dt}\sum_a (\vec{r}_a \times \vec{p}_a) = 0$$

Here is arbitrary rotation $\delta\vec{Q}$, so we conclude that the vector

$$\frac{d}{dt}\sum_a (\vec{r}_a \times \vec{p}_a) = 0 \Rightarrow \sum_a (\vec{r}_a \times \vec{p}_a) = \text{Constant}$$

$$\boxed{\vec{M} \equiv \sum_a \vec{r}_a \times \vec{p}_a} \qquad (2.17)$$

is called the angular momentum of moment of momentum of the system is conserved in motion of the closed system.

- Like the linear momentum, it is additive, whether or not the particles in the system interact.

- There are no other additive integrals of the motions. Thus every system has seven such integrals: energy, three components of momentum, and three components of angular momentum.

Note : $\because$ With respect to origin O angular momentum of the system of particles is $\vec{M} = \sum_a \vec{r}_a \times \vec{p}_a$ where $\vec{r}_a$ is radius vector of a point w.r.t. origin O.

Let $\vec{r}_a'$ be radius vector of the given same point w.r.t. origin O' and distance between O and O' is $\vec{a}$ i.e. $OO' = \vec{a}$

i.e. $\vec{r}_a = \vec{r}_a' + \vec{a}$

$$\therefore \vec{M} = \sum_a (\vec{r}_a' + \vec{a}) \times \vec{p}_a$$

$$= \sum_a \vec{r}_a' \times \vec{p}_a + \sum_a \vec{a} \times \vec{p}_a$$

$$= \sum_a \vec{r}_a' \times \vec{p}_a + \vec{a} \times \left(\sum_a \vec{p}_a \right)$$

$$\boxed{\vec{M} = \vec{M}' + \vec{a} \times \vec{P}} \qquad (2.18)$$

Here $\sum_a \vec{p}_a = \vec{P} = \text{Total linear momentum of the system}$

$\vec{M}'$ = Angular momentum of the system w.r.to origin O′

Since formula (2.18)contains term $\vec{a}$, so the angular momentum depends on the choice of origin except when $\vec{a} \times \vec{p}$ is zero, in that case either system is at rest as a whole $(i.e.\ \vec{p} = 0)$ or $\vec{a}$ and $\vec{p}$ are parallel This indeterminacy, of course, does not affect the law of conservation of angular momentum, since momentum is also conserved in a closed system.

Transformation of Angular momentum from one inertial frame to another:

In K-frame $\vec{M} = \sum_a m_a \vec{r}_a \times \vec{v}_a$

We shall suppose that the origins in the frame K at K' coincide at a given instant. Then the radius vectors of the particle are the same in the two frames, while their velocities are related by eq.(2.4)

$$\vec{v}_a = \vec{v}_a' + \vec{V}$$

Where $\vec{v}_a, \vec{v}_a'$ are the velocities of particle in K and K' frames respectively .Here frame K' moves with velocity $\vec{V}$ with respect to frame K .

$$\vec{M} = \sum_a \vec{r}_a \times \vec{p}_a = \sum_a m_a \vec{r}_a \times \vec{v}_a$$

$$\therefore \quad \vec{M} = \sum_a m_a \vec{r}_a \times \left(\vec{v}_a' + \vec{V}\right)$$

$$= \sum_a m_a \vec{r}_a \times \vec{v}_a' + \sum_a m_a \vec{r}_a \times \vec{V}$$

$$= \vec{M}' + \left(\sum_a m_a \vec{r}_a\right) \times \vec{V}$$

By eq.(2.9)

$$\boxed{\vec{R}_{cm} = \frac{\sum m_a \vec{r}_a}{\sum m_a}} = \frac{\sum m_a \vec{r}_a}{\mu} \Rightarrow \sum m_a \vec{r}_a = \mu \vec{R}_{cm}$$ where μ is the mass of the system

Here $\vec{R}_{cm}$ is the position vector of center of mass of the system of particles with respect to frame K.

$$\therefore \boxed{\vec{M} = \vec{M}' + \mu \vec{R}_{cm} \times \vec{V}} \qquad (2.19)$$

If the K' is the frame in which centre of mass of the system of the particles is considered at rest, then both centre of mass of the system and frame moves with

same velocity $\vec{V}$ and $\mu\vec{V}$ its total momentum of system of particles with respect to frame K i.e. $\mu\vec{V} = \vec{P}$

Thus $\vec{M} = \vec{M}' + \vec{R}_{cm} \times \vec{P}$

$\vec{M}' =$ intrinsic angular momentum

= Angular momentum of the system with respect to origin O′ of the frame K′

$\vec{R}_{cm} \times \vec{P} =$ angular momentum due to its motion as a whole

= Angular momentum of the centre of mass of the system with respect to origin O of the frame K

Note: Although the law of conservation of all three components of angular momentum (relative to an arbitrary origin) is valid only for a closed system, the law of conservation may hold in a more restricted form even for a system in an external field.

It is evident from the above derivation that component of angular momentum only an axis about which the field is symmetrical is always conserved, for the mechanical properties of the system are unaltered by any rotation about that axis. Here the angular momentum must, of course, be defined relative to an origin lying on the axis.

The most important such case is that of a centrally symmetric field (like gravitational field) i.e. one in which the potential energy depends only on the distance from some particular point (the centre). It is evident that the component of angular momentum along any axis passing through the centre is conserved in motion in such a field. In other words, the angular momentum $\vec{M}$ is conserved provided that it is defined w.r.to the centre of the field.

Another examples is that of a homogenous field in the z-direction; in such a field, the component M_z of the angular momentum is conserved, whatever point is taken as the origin.

$\because \boxed{p_\varphi = \frac{\partial L}{\partial \dot{\varphi}}}$

The generalized momentum corresponding to coordinate ϕ is $p_\phi = \dfrac{\partial L}{\partial \dot{\phi}}$ which is basically angular momentum about z axis.

Angular momentum of the system $M_z = \sum p_\phi$

$$\therefore \qquad \boxed{M_z = \sum_a \frac{\partial L}{\partial \dot{\varphi}_a}} \tag{2.20}$$

where the coordinate ϕ is the angle of rotation about z-axis. This is evident from the above proof of the law of conservation of angular momentum, but can also be proved directly :

Using Cartesian coordinates for a single particle , angular momentum

$$\vec{M} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ mv_x & mv_y & mv_z \end{vmatrix}$$

$$\vec{M} = m(yv_z - zv_y)\hat{i} + m(zv_x - xv_z)\hat{j} + m(xv_y - yv_x)\hat{k}$$

$$M_x = m(yv_z - zv_y) = m(y\dot{z} - z\dot{y}) \tag{2.21}$$

$$M_y = m(zv_x - xv_z) = m(z\dot{x} - x\dot{z}) \tag{2.22}$$

$$M_z = m(xv_y - yv_x) = m(x\dot{y} - y\dot{x}) \tag{2.23}$$

Now for system of particles total z component of angular momentum

$$M_z = \sum_a m_a \left(x_a \dot{y}_a - y_a \dot{x}_a\right)$$

In cylindrical coordinates

$$\begin{cases} \boxed{x = r\cos\varphi \ , \quad y = r\sin\varphi \ , \quad z = z} \\ \dot{x} = \dot{r}\cos\varphi - r\sin\varphi\dot{\varphi} \ , \quad \dot{y} = \dot{r}\sin\varphi + r\cos\varphi\dot{\varphi} \ , \quad \dot{z} = \dot{z} \end{cases} \tag{2.24}$$

Putting these values in expression of M_z

$$\Rightarrow M_z = m[r\cos\phi(\dot{r}\sin\phi + r\cos\phi\dot{\phi}) - r\sin\phi(\dot{r}\cos\phi - r\sin\phi\dot{\phi})]$$

$$\Rightarrow \boxed{M_z = \sum_a m_a r_a^2 \dot{\varphi}_a} \tag{2.25}$$

The Lagrangian is, in terms of r , ϕ , z , is

$$L = \frac{1}{2}\sum_a m_a\left(\dot{r}_a^2 + r_a^2\dot{\varphi}_a^2 + \dot{z}_a^2\right) - U \qquad (2.26)$$

In cylindrical coordinates velocity of a particle is given by

$$\boxed{v = \sqrt{\left(\dot{r}_a^2 + r_a^2\dot{\varphi}_a^2 + \dot{z}_a^2\right)}}$$

Here potential energy U is independent of velocity coordinates $\dot{r}, \dot{\phi}, \dot{z}$

Using eq.(2.20) $M_z = \sum_a \frac{\partial L}{\partial \dot{\phi}_a}$

We have $M_z = \sum_a \frac{\partial}{\partial \dot{\phi}_a}\left\{\frac{1}{2}\sum_a m_a\left(\dot{r}_a^2 + r_a^2\dot{\phi}_a^2 + \dot{z}_a^2\right) - U\right\}$

$$M_z = \sum_a \left\{\frac{1}{2}\sum_a m_a\left(0 + r_a^2 2\dot{\phi}_a + 0\right) - 0\right\}$$

$M_z = \sum_a m_a r_a^{\,2}\dot{\phi}_a$ which is the same result as we have obtained in eq(2.25)

Example 2.4 Express M_x, M_y, M_z of a particle in cylindrical coordinates

Sol. By eq.(2.24) $x = r\cos\phi$, $y = r\sin\phi$, $z = z$

$\dot{x} = \dot{r}\cos\phi - r\sin\phi\dot{\phi}$, $\dot{y} = \dot{r}\sin\phi + r\cos\phi\dot{\phi}$, $\dot{z} = \dot{z}$

By eq.(2.21)

$$M_x = yp_z - zp_y$$
$$= r\sin\phi\, m\,\dot{z} - z.m\left(\dot{r}\sin\phi + r\cos\phi\dot{\phi}\right)$$
$$= m\sin\phi\left(r\dot{z} - z\dot{r}\right) - m\,r\,z\,\dot{\phi}\cos\phi$$

By eq.(2.22)

$$M_y = zp_x - xp_z$$
$$= m(z\dot{x} - x\dot{z})$$
$$= m[z(\dot{r}\cos\phi - r\sin\phi\dot{\phi}) - r\cos\phi\,\dot{z}]$$

By eq.(2.22) $M_z = xp_y - yp_x$

$$= m[r\cos\phi(\dot{r}\sin\phi + r\cos\phi\dot{\phi}) - r\sin\phi(\dot{r}\cos\phi - r\sin\phi\dot{\phi})]$$
$$= mr^2\dot{\phi}$$

Example 2.5 Express M_x, M_y, M_z of a particle in spherical coordinates r, θ, ϕ

Sol. In spherical coordinates

$$\boxed{x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta}$$

$$\Rightarrow \dot{x} = \dot{r}\sin\theta\cos\phi + r\cos\theta\cos\phi\dot{\theta} - r\sin\theta\sin\phi\dot{\phi}$$

$$\Rightarrow \dot{y} = \dot{r}\sin\theta\sin\phi + r\cos\theta\sin\phi\dot{\theta} + r\sin\theta\cos\phi\dot{\phi}$$

$$\Rightarrow \dot{z} = \dot{r}\cos\theta - r\sin\theta\dot{\theta}$$

By eq.(2.21)

$$M_x = yp_z - zp_y = r\sin\theta\sin\varphi.m\left(\dot{r}\cos\theta - r\sin\theta\dot{\theta}\right)$$
$$- r\cos\theta.m.\left(\dot{r}\sin\theta\sin\varphi + r\cos\theta\sin\varphi\dot{\theta} + r\sin\theta\cos\varphi\dot{\varphi}\right)$$
$$= -mr^2\left(\dot{\theta}\sin\phi\right) - mr^2\sin\theta\cos\theta\cos\phi\dot{\phi}$$

By eq.(2.22)

$$M_y = zp_x - xp_z$$
$$= m(z\dot{x} - x\dot{z})$$
$$= m[(r\cos\theta)(\dot{r}\sin\theta\cos\varphi + r\cos\theta\cos\varphi\dot{\theta} - r\sin\theta\sin\varphi\dot{\varphi})$$
$$- (r\sin\theta\cos\varphi)(\dot{r}\cos\theta - r\sin\theta\dot{\theta})]$$
$$= mr^2[\dot{\theta}\cos\phi - \dot{\phi}\sin\theta\cos\theta\sin\phi]$$

By eq.(2.23)

$$M_z = xp_y - yp_x$$
$$= m[x\dot{y} - y\dot{x}]$$
$$= m[r\sin\theta\cos\phi(\dot{r}\sin\theta\sin\phi + r\cos\theta\sin\phi\dot{\theta} + r\sin\theta\cos\phi\dot{\phi}) -$$
$$r\sin\theta\sin\phi(\dot{r}\sin\theta\cos\phi + r\cos\theta\cos\phi\dot{\theta} - r\sin\theta\sin\phi\dot{\phi})]$$
$$= mr^2\dot{\phi}\sin^2\theta$$

Example 2.6 Which components of momentum $\vec{P}$ and momentum $\vec{M}$ are conserved in motion in the following fields?

(a) The field of an infinite homogeneous plane
(b) That of an infinite homogeneous cylinder
(c) That of an infinite homogeneous prism

(d) That of two points

(e) That of an infinite homogeneous half-plane

(f) That of a homogeneous cone

(g) That of a homogeneous circular torus

(h) That of an infinite homogeneous cylindrical helix

Sol.(a) P_x, P_y, M_z if the is $x-y$ plane

(b) P_z, M_z, if z is the axis of cylinder.

(c) P_z, if the edges of the prism are parallel to the z-axis.

(d) M_z (if the line joining the point is the z-axis).

(e) P_y (if the edge of the half plane is y-axis).

(f) M_z, if the axis of the cone is the z-axis.

(g) M_z (if the axis of the torus is z-axis).

(h)Let b be the pitch of the helix, we can write for change in Lagrangian

$$\delta L = \frac{\partial L}{\partial z}\delta z + \frac{\partial L}{\partial \phi}\delta\phi \equiv 0 \text{ (homogeneity of space under translation and rotation)}$$

$$\delta L = \left\{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{z}}\right)\right\}\delta z + \left\{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\phi}}\right)\right\}\delta\phi = 0$$

$$\Rightarrow \left\{\frac{d}{dt}\left(p_z\right)\right\}\delta z + \left\{\frac{d}{dt}\left(p_\phi\right)\right\}\delta\phi = 0$$

$$\left[\because p_z = \left(\frac{\partial L}{\partial \dot{z}}\right), p_\phi = \left(\frac{\partial L}{\partial \dot{\phi}}\right)\right]$$

$$\Rightarrow \left\{\frac{d}{dt}\left(p_z\right)\right\}\delta z + \left\{\frac{d}{dt}\left(M_z\right)\right\}\delta\phi = 0 \qquad [\because M_z = p_\phi]$$

$$\Rightarrow \frac{dp_z}{dt}\delta z + \frac{dM_z}{dt}\delta\phi = 0$$

$$\left(\because A\text{fter one revolution change in z is b andchange in } \phi \text{ is } 2\pi \text{ ,So } \frac{b}{2\pi} = \frac{\delta z}{\delta\phi}\right)$$

$$\Rightarrow \frac{dp_z}{dt}\delta z + \frac{dM_z}{dt}\frac{2\pi}{b}\delta z = 0$$

$$\Rightarrow \delta z.\frac{d}{dt}\left(P_z+\frac{2\pi}{b}M_z\right)=0$$

Since δz is arbitrary therefore

$$\frac{d}{dt}\left(P_z+\frac{2\pi}{b}M_z\right)=0 \qquad \because P_z+\frac{2\pi}{b}M_z=\text{Constant}$$

2.6 Summary

We have derived the laws of conservation of energy, momentum, and angular momentum on the basis of invariance of Lagrangian under translation in time, translation in space and isotropy of space respectively. We have followed the Lagrangian approach which is very powerful in higher physical problem solving.

2.7 Glossary

***Homogeneous*:** consisting of parts that are similar to each other or are of the same type

Indeterminate: not measured, counted, or clearly known:

2.8 Answer to Self Learning Exercise

Ans.1: C

2.9 Exercise

Q.1 Which component of momentum $\vec{P}$ and angular momentum $\vec{M}$ are conserved in the field of an infinite homogeneous cylinder, if z is the axis of the cylinder.

(A) P_z only (B) M_z only

(C) P_z and M_z both (D) Neither P_z nor M_z

Q.2 Define the angular momentum.

Q.3 What are "Integrals of Motion" ?

Q.4 Show that if the Lagrangian does not depend explicitly on the time, then the energy is conserved.

Q.5 Prove the laws of conservation of linear momentum energy for a system of interacting particles.

2.10 Answers to Exercise

Ans.1: C

Ans.3: See the Text

References and Suggested Readings

1. L.D. Landau and E. M. Lifshitz, Mechanics, Butterworth- Heinemann

2. Gupta ,Kumar &Sharma ,Classical Mechanics, Pragati Prakashan Meerut , 1998

3. Goldstein, Poole &Saiko, Classical Mechanics, Pearson Education 2002

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UNIT-3
Integration of the Equations of Motion

Structure of the Unit

3.0 Objectives

3.1 Introduction

3.2 Motion in One Dimension

3.3 The Two Body Problem : The Reduced Mass

3.4 Motion in a Central Field

3.5 Self Learning Exercise-I

3.6 Kepler's Problem

3.7 Self Learning Exercise-II

3.8 Summary

3.9 Glossary

3.10 Answers to Self Learning Exercises

3.11 Exercise

3.12 Answers to Exercise

References and Suggested Reading

3.0 Objectives

In this chapter we shall focus upon the motion of a dynamical system having one degree of freedom. Specifically we shall focus upon the following topics :

- Lagrangian of a one dimension motion of a particle.
- Obtaining first order differential equations from the law of conservation of energy.
- Turning points of the motion and potential energy diagram.
- Simple examples of motion in one dimension.
- The two body problem.

- Motion in a central field.
- Fall of a particle to the central of force.
- Kepler's problem.

3.1 Introduction

In one dimension motion of a particle it is not necessary to write equation of motion. In one dimension motion ,we can start from the first integral of the Lagrangian equation i.e. the law of conservation of energy. This gives first-order differential equation, which can be integrated immediately. Since the kinetic energy is essentially positive, the total energy always exceeds the potential energy, i.e. the motion can take place only in those regions of space where the potential energy is less than the total energy. The points at which the potential energy equals the total energy give the limits of the motion. We shall integrate the equations of motion in general form for the motion of a particle in central field, Kepler's problem etc.

3.2 Motion in One Dimension

The motion of a system having one degree of freedom is said to take place in *one dimension*. The most general form of the Lagrangian of such a system in fixed external conditions is

$$L = \frac{1}{2} a(q)\dot{q}^2 - U(q) \qquad \text{(a)}$$

where $a(q)$ is some function of the generalized co-ordinate q. In particular, if q is a Cartesian co-ordinate (x, say) then

$$L = \frac{1}{2} m\dot{x}^2 - U(x) \ . \qquad \text{(b)}$$

We can start from the first integral of this equation, which gives the law of conservation of energy. For the Lagrangian (b) we have

$$\frac{1}{2} m\dot{x}^2 - U(x) = E$$

This is a first-order differential equation, and can be integrated immediately. Since

$$\frac{dx}{dt} = \sqrt{\frac{2}{m}(E - U(x))} \quad , \text{ it follows that}$$

$$t = \sqrt{\left(\frac{1}{2}m\right)} \int \frac{d\,x}{\sqrt{(E - U\,(x))}} + \text{constant}$$

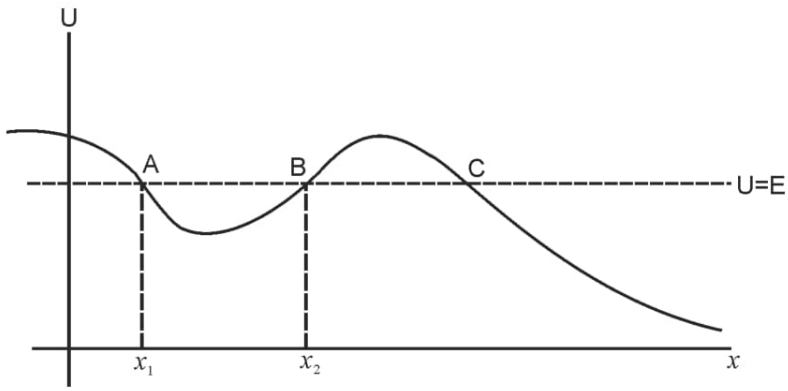


Figure 3.1

The two arbitrary constants of motion are here represented by total energy E and the constant of integration. Since the kinetic energy is essentially positive, the total energy is always exceeds the potential energy i.e. the motion can take place only in those regions of space where $U\,(x) < E$. The points at which the potential energy equals the total energy $U\,(x) = E$

give the limits of the motion, they are the turning points of the motion, since the velocity there is zero. if the region of the motion is bounded by two such points, then the motion takes place in a finite region of space, and is said to be finite. If the region of motion is limited on only one side , or on neither , then the motion is infinite and the particle goes to infinity.

A finite motion in one dimension is oscillatory, the particle moving repeatedly back and forth between two points x_1 and x_2. The period T of the oscillations, i.e. the time during which the particle passes from x_1 to x_2 and back , is twice the time from x_1 to x_2 :

$$T\,(E) = \sqrt{(2\,m)} \int_{x_1(E)}^{x_2(E)} \frac{d\,x}{\sqrt{(E - U\,(x))}}$$

where x_1 and x_2 are the roots of equation (4) for the given value of E.

3.3 The Two Body Problem : (The Reduced Mass)

We consider a system consisting of two interacting particles (the two body problem). The motion of two interacting particles can be reduced to that of one

particle system as follows. As a first step towards the solution of this problem, we shall show how it can be considerably simplified by separating the motion of the system into the motion of the centre of mass and that of particles relative to the centre of mass.

Let $\vec{r}_1$ be the position vector of particle m_1 and let $\vec{r}_2$ be the position vector of the particle 2 of mass m_2.

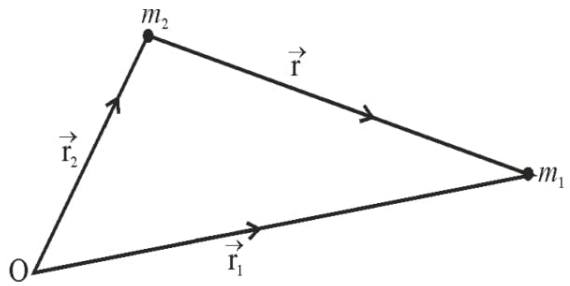


Figure 3.2

The potential energy of the interaction of two particles depends only on the distance between them. The Lagrangian of such a system is therefore

$$L = T - U$$

or
$$\boxed{L = \frac{1}{2} m_1 \dot{\vec{r}}_1^{\,2} + \frac{1}{2} m_2 \dot{\vec{r}}_2^{\,2} - U\left(|\vec{r}_1 - \vec{r}_2|\right)} \qquad (3.1)$$

Let
$$\vec{r} = \vec{r}_1 - \vec{r}_2 \qquad (3.2)$$

be the relative position vector, and let the origin be at the centre of mass,

$$r_{CM} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} = \vec{0} \text{ i.e. } m_1 \vec{r}_1 + m_2 \vec{r}_2 = \vec{0} \quad , \qquad (3.3)$$

solving (3.2) and (3.3) we get, $\vec{r}_1 = \frac{m_2 \vec{r}}{m_1 + m_2}$, $\vec{r}_2 = -\frac{m_1 \vec{r}}{m_1 + m_2}$ (3.4)

Substituting in (3.1), we get

$$L = \frac{1}{2} m_1 \frac{m_2^2}{(m_1 + m_2)^2} \dot{\vec{r}}^{\,2} + \frac{1}{2} m_2 \frac{m_1^2}{(m_1 + m_2)^2} \dot{\vec{r}}^{\,2} - U(|\vec{r}_1 - \vec{r}_2|)$$

$$\text{or } L = \frac{1}{2} \frac{m_1 m_2}{(m_1 + m_2)^2} \dot{\vec{r}}^{\,2} - U(r) \text{ where } r = |\vec{r}_1 - \vec{r}_2|$$

$$\Rightarrow \boxed{L = \frac{1}{2} m \dot{\vec{r}}^2 - U(r)}, \text{ where } m = \frac{m_1 m_2}{m_1 + m_2}$$

i.e. the Lagrangian of two interacting particles can be reduced to the of one particle having mass $\boxed{m = \frac{m_1 m_2}{m_1 + m_2}}$, this mass m is called ***reduced mass.***

3.4 Motion in a Central Field

On reducing the two-body problem to one of the motion of a single body, we arrive at the problem of determining the motion of a single particle in an external field such that its ***potential energy depends only on the distance*** r ***from some fixed points. This is called a central field.***

The force acting on the particle is

$\boxed{\vec{F} = -\frac{\partial U(r)}{\partial \vec{r}} = -\left(\frac{dU}{dr}\right)\frac{\vec{r}}{r} = -\frac{dU}{dr}\hat{r}}$; its magnitude is a function of r only, and its direction is everywhere that of the radius vector. So torque

$$\vec{\tau} = \vec{r} \times \vec{F} = \vec{r} \times \left(-\frac{dU}{dr}\hat{r}\right) = 0$$

$\because \vec{\tau} = \frac{d\vec{M}}{dt} = 0$ ***therefore angular momentum*** $\vec{M}$ ***of the system relative to the centre of such a field is conserved.***

$\because$ $\vec{M} = \vec{r} \times \vec{p}$, the constancy of $\vec{M}$ shows that, therefore the motion, the radius vector of the particle lies in the plane perpendicular to $\vec{M}$. Thus the path of a particle in a central field lies in one plane. In polar coordinate velocity of the particle is $\boxed{\sqrt{\dot{r}^2 + r^2\dot{\varphi}^2}}$

The Lagrangian is

$$L = \frac{1}{2} m\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - U(r) \qquad (3.4)$$

Since $\frac{\partial L}{\partial \phi} = 0 = \dot{p}_\phi$

$\therefore \phi$ ***is cyclic coordinate and generalized momentum*** p_ϕ ***is constant*** ,

$P_\phi = \dfrac{\partial L}{\partial \dot{\phi}} = \dfrac{1}{2} m r^2 2\dot{\phi} = m r^2 \dot{\phi} =$ ***Constant . This generalized momentum*** p_ϕ ***is basically angular momentum of the particle. i.e***

. $\boxed{M = m r^2 \dot{\varphi}} = \text{constant}$ (3.5)

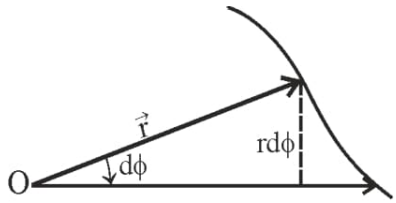


Figure 3.3

We can express (3.5) as

$$M = m r^2 \frac{d\phi}{dt}$$

$$\Rightarrow M = 2m\dot{f} \tag{3.6}$$

(where $\dot{f} = \dfrac{1}{2} r^2 \dfrac{d\phi}{dt}$ and $\dot{f}$ is called the sectorial velocity.)

The complete solution of the problem of the motion of a particle in a central field is most easily obtained by starting from the laws of conservation of energy and angular momentum, without using equation of motion

We write Total energy E = T+U

$$\Rightarrow E = \frac{1}{2} m\left(\dot{r}^2 + r^2\dot{\phi}^2\right) + U(r)$$

By eq.(3.5) ,putting $\dot{\phi} = \dfrac{M}{m r^2}$ in above equation ,we get

$$E = \frac{1}{2} m\dot{r}^2 + \frac{M^2}{2mr^2} + U(r) \tag{3.7}$$

Hence $\dot{r} \equiv \dfrac{dr}{dt} = \sqrt{\left\{\dfrac{2}{m}\{E - U(r)\} - \dfrac{M^2}{m^2 r^2}\right\}}$ (3.8)

$$\Rightarrow dt = \frac{dr}{\sqrt{\left\{\dfrac{2}{m}\{E - U(r)\} - \dfrac{M^2}{m^2 r^2}\right\}}}$$

On integrating above expression

$$t = \int \frac{dr}{\sqrt{\left\{\frac{2}{m}\left[E - U(r)\right] - \frac{M^2}{m^2 r^2}\right\}}} + \text{Constant} \qquad (3.9)$$

From eq.(3.5) $\dot{\phi} = \frac{M}{mr^2}$ or Writing $d\phi = \frac{Mdt}{mr^2}$, or $dt = \frac{mr^2 d\phi}{M}$ substituting dt in eq. (3.8), we find

$$d\phi = \frac{Mdr}{mr^2\sqrt{\left\{\frac{2}{m}\left[E - U(r)\right] - \frac{M^2}{m^2 r^2}\right\}}}$$

$$\Rightarrow d\phi = \frac{\frac{Mdr}{r^2}}{\sqrt{\left\{2m\left[E - U(r)\right] - \frac{M^2}{r^2}\right\}}}$$

$$\text{Or} \quad \varphi = \int \frac{Mdr/r^2}{\sqrt{\left\{2m\left[E - U(r)\right] - \frac{M^2}{r^2}\right\}}} + \text{Constant} \qquad (3.10)$$

Formulae (3.9) and (3.10) give the general solution of the problem. Eq. (3.10) gives the equation of the path.

It should be noted that the angle ϕ always varies monotonically with line, since (3.5) shows that $\dot{\phi}$ can never change sign.

The expression (3.7) i.e. $\boxed{E = \frac{1}{2}m\dot{r}^2 + \frac{M^2}{2mr^2} + U(r)}$ shows that the radial part of the motion can be regarded as taking place in one dimension in a field when the "effective potential energy" is

$$\boxed{U_{eff} = U(r) + \frac{M^2}{2mr^2}} \qquad (3.11)$$

The term $\frac{M^2}{2mr^2}$ is called the centrifugal potential energy.

For maxima and minima of r , derivative $\dot{r}$ becomes zero. The values of r for which

$$U(r)+\frac{M^2}{2mr^2}=E \qquad (3.12)$$

determines the limits of the motion as regards distance from the centre.

When equation (3.12) is satisfied, the radial velocity $\dot{r}$ is zero. This does not mean that the particle comes to rest as in true one dimensional motion, since the angular velocity $\dot{\phi}$ is not zero.

The value $\dot{r}=0$ indicates a turning point of the path, where increasing $r(t)$ begins to decrease or decreasing $r(t)$ begins to increase.

If the range in which r may vary is limited only by the condition $r \geq r_{min}$, the motion is infinite: the particle comes from, and returns to, infinity.

If the range of r has two limits r_{min} and r_{max} the motion is finite and the path lies entirely within the annulus bounded by the circles $r=r_{max}$ and $r=r_{min}$.

This does not mean, however, that the path must be a closed curve(Closed curve means particle returns to its initial position) .

During the time in which r varies from r_{max} to r_{min} and back(i.e. r_{min} to r_{max}), the radius vector turns through an angle $\Delta\phi$ which, according to (3.10), is given by

$$\Delta\varphi = 2\int_{r_{min}}^{r_{max}} \frac{M dr/r^2}{\sqrt{2m(E-U)-\frac{M^2}{r^2}}}$$

(3.13) The condition for the path to be closed is that this angle should be a rational fraction of 2π i.e., that $\Delta\phi = 2\pi.\frac{m}{n}$, or $n\Delta\phi = 2\pi\, m$ where m and n are integers. In that case, after n periods(period means r_{max} to r_{min} and then r_{min} to r_{max}), the radius vector of the particle will have made m complete revolutions and will occupy, its original position, so that the path is closed.

Such cases as exceptional, however, and when the form of $U(r)$ is arbitrary the angle $\Delta\phi$ is not a rational fraction of 2π . In general, therefore, the path of a particle executing a finite motion is not closed.

It passes through the minimum and maximum distances an infinity of times, and after infinite times covers the entire annulus between the two bounding circles.

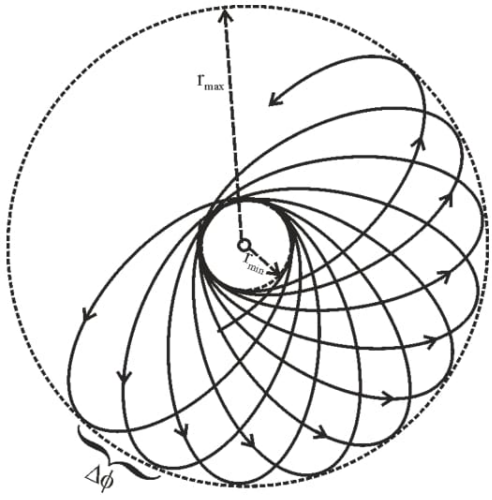


Figure 3.4

There are only two types of central field in which all finite motions take place in closed paths. They are those in which the potential energy of the particle varies as $\frac{1}{r}$ or as r^2.

Important Note: The presence of the centrifugal energy when $M \neq 0$, which becomes infinite as $\frac{1}{r^2}$ when $r \to 0$, generally renders its impossible for the particle to reach the centre of the field, even if the field is an attractive one. A "fall" of the particle to the centre is possible only if the potential energy tends sufficiently rapidly to $-\infty$ as $r \to 0$. From (3.7) the inequality

$$\frac{1}{2}m\dot{r}^2 = E - U(r) - \frac{M^2}{2mr^2} > 0$$

$$\text{or } r^2U(r) + \frac{M^2}{2m} < Er^2,$$

It follows that r can take values tending to zero only if

$$\left[r^2U(r) + \frac{M^2}{2m}\right]_{\lim r\to 0} < \left[Er^2\right]_{\lim r\to 0}$$

$$\Rightarrow \left[r^2U(r)\right]_{\lim r\to 0} + \frac{M^2}{2m} < 0 \qquad \left\{\because \left[Er^2\right]_{\lim r\to 0} \cong 0\right\}$$

$$\Rightarrow \left[r^2 U(r)\right]_{\lim r\to 0} < -\frac{M^2}{2m}$$

i.e. $U(r)$ must tend to $-\infty$ either as $-\frac{\alpha}{r^2}$ with $\alpha > \frac{M^2}{2m}$, or proportionally to $-\frac{1}{r^n}$ with $n > 2$.

Example 3.1 Determine the period of oscillations of a simple pendulum (a particle of mass *m* suspended by a string of length l in a gravitational field) as a function of the amplitude of the oscillations.

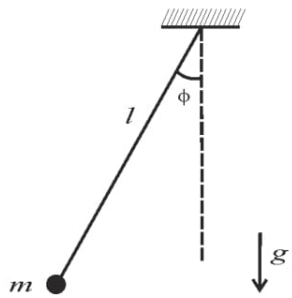


Figure 3.5

Total energy of the system $E = \frac{1}{2}mv^2 + U$

Potential energy $U = -\vec{F}.\vec{r} = -mgl\cos\phi$

Arc element $ds = ld\phi \;\therefore v = \frac{ds}{dt} = l\frac{d\phi}{dt} = l\dot{\phi}$

$$E = \frac{1}{2}ml^2\dot{\varphi}^2 - mgl\cos\varphi \qquad (3.14)$$

Total energy of system remains constant. When particle is at extreme position its velocity becomes zero and it has only potential energy that will be equal to its total energy.

$$\because\; E = -mgl\cos\varphi_0 \qquad (3.15)$$

where ϕ_0 : initial angular displacement or angular amplitude

Therefore we express (3.14), by making use of (3.15) as

$$-mgl\cos\phi_0 = \frac{1}{2}ml^2\dot{\phi}^2 - mgl\cos\phi$$

$$\text{or } \frac{1}{2}ml^2\dot{\phi}^2 = mgl[\cos\phi - \cos\phi_0]$$

$$= mgl\left[\left(1-2\sin^2\frac{\phi}{2}\right)-\left(1-2\sin^2\frac{\phi_0}{2}\right)\right]$$

$$= mgl\left[2\sin^2\frac{\phi_0}{2}-2\sin^2\frac{\phi}{2}\right]$$

$$\therefore \quad \dot{\phi}^2 = \frac{mgl.2}{\frac{1}{2}ml^2}\left[\sin^2\frac{\phi_0}{2}-\sin^2\frac{\phi}{2}\right]$$

$$\Rightarrow \dot{\phi}^2 = 4\frac{g}{l}\left[\sin^2\frac{\phi_0}{2}-\sin^2\frac{\phi}{2}\right]$$

$$\Rightarrow \dot{\phi} = 2\sqrt{\frac{g}{l}}\left(\sin^2\frac{\phi_0}{2}-\sin^2\frac{\phi}{2}\right)^{\frac{1}{2}}$$

$$\therefore \quad dt = \frac{d\phi}{2\sqrt{\frac{g}{l}}\sqrt{\sin^2\frac{\phi_0}{2}-\sin^2\frac{\phi}{2}}}$$

Let time period of oscillation is T. When ϕ varies from 0 to ϕ_0 and corresponding to it time taken is $\frac{T}{4}$

$$\therefore \frac{T}{4} = \frac{1}{2}\sqrt{\frac{l}{g}}\int_0^{\phi_0}\frac{d\phi}{\sqrt{\sin^2\frac{\phi_0}{2}-\sin^2\frac{\phi}{2}}}$$

$$\Rightarrow T = 2\sqrt{\frac{l}{g}}\int_0^{\varphi_0}\frac{d\varphi}{\sqrt{\sin^2\frac{\varphi_0}{2}-\sin^2\frac{\varphi}{2}}} \tag{3.16}$$

Let $$\frac{\sin\frac{\varphi}{2}}{\sin\frac{\varphi_0}{2}} = \sin\xi \tag{3.17}$$

Differentiating above expression

$$\therefore \frac{1}{\sin\frac{\phi_0}{2}}.\frac{1}{2}\cos\frac{\phi}{2}d\phi = \cos\xi\, d\xi$$

$$\therefore d\varphi = \frac{2\sin\frac{\varphi_0}{2}}{\cos\frac{\varphi}{2}}.\cos\xi\, d\xi \tag{3.18}$$

From (3.16),(3.17) and (3.18) we have

$$\therefore T = 2\sqrt{\frac{l}{g}}\int\left(\frac{2\sin\frac{\varphi_0}{2}.\cos\xi\, d\xi}{\cos\frac{\varphi}{2}.\sin\frac{\varphi_0}{2}\sqrt{1-\sin^2\xi}}\right)$$

$$\Rightarrow T = 4\sqrt{\frac{l}{g}}\int\frac{\cos\xi}{\cos\frac{\phi}{2}\cos\xi}d\xi = 4\sqrt{\frac{l}{g}}\int\frac{d\xi}{\cos\frac{\phi}{2}}$$

From(3.17) , $\dfrac{\sin\frac{\phi}{2}}{\sin\frac{\phi_0}{2}} = \sin\xi$ When $\begin{cases}\phi = 0 \Rightarrow \sin\xi = 0, \xi = 0\\ \phi = \phi_0 \Rightarrow \sin\xi = 1, \xi = \dfrac{\pi}{2}\end{cases}$

Also $\sin\dfrac{\phi}{2} = \sin\xi\sin\dfrac{\phi_0}{2}$ or $\cos\dfrac{\phi}{2} = \sqrt{1-\sin^2\xi\sin^2\dfrac{\phi_0}{2}}$

Using these facts for expression of time period T, We get

$$T = 4\sqrt{\frac{l}{g}}\int_0^{\frac{\pi}{2}}\frac{d\xi}{\sqrt{1-\sin\frac{\phi_0}{2}.\sin^2\xi}}$$

$$\Rightarrow T = 4\sqrt{\frac{l}{g}}\,K\left(\sin\frac{\varphi_0}{2}\right) = 4\sqrt{\frac{l}{g}}\,K(k) \tag{3.19}$$

where $k = \sin\dfrac{\phi_0}{2}$

$K(k) = \displaystyle\int_0^{\frac{\pi}{2}}\frac{d\xi}{\sqrt{1-k^2\sin^2\xi}}$ is the complete elliptic integral of the first kind.

For small oscillations $\phi_0 << 1, \phi << 1,\ \sin\frac{\varphi_0}{2} \approx \frac{1}{2}\varphi_0$ *and* $\sin\frac{\varphi}{2} \approx \frac{1}{2}\varphi$

From eq.(3.16) $T = 2\sqrt{\frac{l}{g}} \int_0^{\phi_0} \frac{d\phi}{\sqrt{\left(\frac{\phi_0}{2}\right)^2 - \left(\frac{\phi}{2}\right)^2}}$

$$= 4\sqrt{l/g} \int_0^{\phi_0} \frac{d\phi}{\sqrt{\phi_0^2 - \phi^2}} = 4\sqrt{\frac{l}{g}} \sin^{-1}\left(\frac{\phi}{\phi_0}\right)\Big|_0^{\phi_0}$$

$$= 4\sqrt{\frac{l}{g}} \left\{\sin^{-1}(1) - \sin^{-1}(0)\right\} = 4\sqrt{\frac{l}{g}}\frac{\pi}{2}$$

$$T = 2\pi\sqrt{l/g}$$

Time period as a function of angular amplitude ϕ_0 :

From eq.(3.19) , $K(k) = \int_0^{\frac{\pi}{2}} \frac{d\xi}{\sqrt{1 - k^2\sin^2\xi}} = \int_0^{\frac{\pi}{2}} \left(1 - k^2\sin^2\xi\right)^{-1/2} d\xi$

As $k = \sin\frac{\phi_0}{2}$ is small for small ϕ_0, For small $k^2\sin^2\xi$,by using binomial theorem

$$K(k) \cong \int_0^{\frac{\pi}{2}} \left(1 + \frac{1}{2}k^2\sin^2\xi + ...\right) d\xi$$

$$= \int_0^{\frac{\pi}{2}} \left(1 + \frac{1}{2}k^2\frac{(1 - \cos 2\xi)}{2}\right) d\xi$$

$$= \int_0^{\frac{\pi}{2}} \left(1 + \frac{1}{4}k^2 - \frac{k^2}{4}\cos 2\xi\right) d\xi$$

$$= \left[\xi + \frac{1}{4}k^2\xi - \frac{k^2}{4.2}\sin 2\xi\right]_0^{\frac{\pi}{2}}$$

$$= \left[\frac{\pi}{2} + \frac{1}{4}k^2 \frac{\pi}{2} - \frac{k^2}{4.2}\sin\pi - 0 \right]_0^{\frac{\pi}{2}}$$

$$\Rightarrow K(k) = \frac{\pi}{2}\left(1 + \frac{k^2}{4}\right)$$

Using $k = \sin\frac{\phi_0}{2} \approx \frac{\phi_0}{2}$ We have $K(k) = \frac{\pi}{2}\left(1 + \frac{\phi_0^{\,2}}{16}\right)$

From eq.(3.19) $T = 4\sqrt{\frac{l}{g}}\,K(k) = 4\sqrt{\frac{l}{g}}\frac{\pi}{2}\left(1 + \frac{\phi_0^{\,2}}{16}\right)$

$$\Rightarrow T = 2\pi\sqrt{\frac{l}{g}}\left(1 + \frac{1}{16}\phi_0^2\right)$$

This is the most famous formula of time period of simple pendulum for large angle approximation .

3.5 Self Learning Exercise-I

Section A : Very Short Answer Type Questions

Q.1 Define Central field.

Q.2 Show that angular momentum of a particle in central field in conserved.

Q.3 Write the Lagrangian of a particle in central field using polar coordinates (r,ϕ) in the plane

Q.4 What are "Turning points" of the motion? If the motion is in a field where the potential energy of the particle is $U = \frac{1}{2}kx^2$, what are the turning points. The energy of the particle E is conserved.

Q.5 Write the Lagrangian of a system of two interacting particles (the two body problem)

Section B : Short Answer Type Questions

Q.6 Find the angular momentum of a particle moving in a central field. Show that ϕ is cyclic coordinate.

Q.7 Let $\vec{r} = \vec{r_1} - \vec{r_2}$ be the relative position vector of the two interacting particles, and origin be chosen at the centre of mass then find $\vec{r_1}, \vec{r_2}$ and L in terms of reduced mass $m = \dfrac{m_1 m_2}{m_1 + m_2}$ and $\vec{r}$.

$$L = \frac{1}{2} m \dot{\vec{r}}^2 - U(\vec{r})$$

Example 3.2 Obtain the expression of the equations of motion for a spherical pendulum in terms of $d\theta$ and dt (a particle of mass m moving on the surface of a sphere of radius l in a gravitational field).

Sol. In spherical coordinates, with the origin at the centre of the sphere and the polar axis vertically downwards, the Lagrangain of the pendulum is

$$L = T - U$$

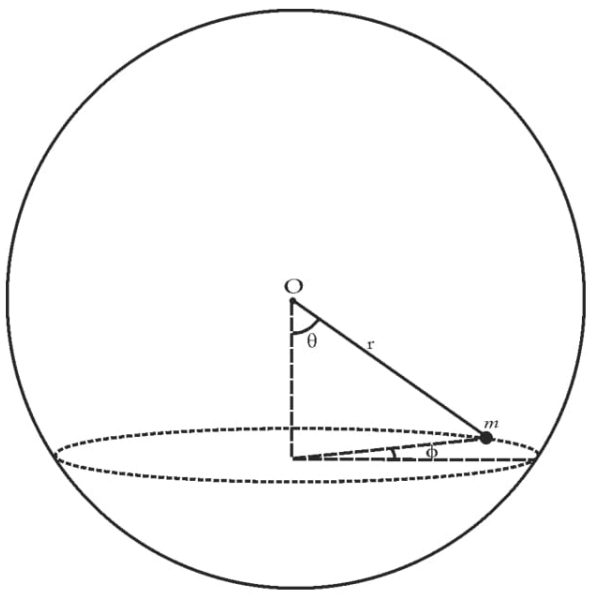


Figure 3.6

In polar coordinates velocity of the particle is

$$\boxed{v = \sqrt{\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta\,\dot{\varphi}^2}} \quad \because r = l = \text{constant}, \therefore \dot{r} = 0$$

$$\therefore \; v = \sqrt{r^2\dot{\theta}^2 + r^2 \sin^2\theta\,\dot{\varphi}^2}$$

$$\therefore L = \frac{1}{2}m\left(l^2\dot{\theta}^2 + l^2\sin^2\theta\,\dot{\varphi}^2\right) + mgl\cos\theta \qquad (3.20)$$

Here $\dot{p}_\phi = \frac{\partial L}{\partial \phi} = 0$ so co-ordinate ϕ is cyclic, and hence the generalized momentum P_ϕ, which is the same as the z-component of angular momentum, is conserved(as ϕ is measured in xy plane) $p_\phi = \frac{\partial L}{\partial \dot{\phi}} =$ Constant .By (3.20)

$$p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = ml^2\sin^2\theta\,\dot{\varphi} = M_z = \text{Constant} \qquad (3.21)$$

Total energy E=T+U

$$\Rightarrow E = \frac{1}{2}m\left(l^2\dot{\theta}^2 + l^2\sin^2\theta\,\dot{\phi}^2\right) - mgl\cos\theta$$

From (3.21) , $\dot{\phi} = \frac{M_z}{ml^2\sin^2\theta}$

Putting this value in the expression of E

$$\text{or } E = \frac{1}{2}ml^2\dot{\theta}^2 + \frac{1}{2}ml^2\sin^2\theta\left(\frac{M_z}{ml^2\sin^2\theta}\right)^2 - mgl\cos\theta$$

$$\Rightarrow E = \frac{1}{2}ml^2\dot{\theta}^2 + \frac{1}{2}\frac{M_z^2}{ml^2\sin^2\theta} - mgl\cos\theta$$

$$\Rightarrow \frac{1}{2}ml^2\dot{\theta}^2 = E - \frac{1}{2}\frac{M_z^2}{ml^2\sin^2\theta} + mgl\cos\theta$$

$$\Rightarrow \dot{\theta}^2 = \frac{2}{ml^2}\left\{E - \frac{1}{2}\frac{M_z^2}{ml^2\sin^2\theta} + mgl\cos\theta\right\}$$

$$dt = \frac{d\theta}{\sqrt{\frac{2}{ml^2}\left(E - \frac{1}{2}\frac{M_z^2}{ml^2\sin^2\theta} + mgl\cos\theta\right)}}$$

3.6 Kepler's Problem

An important class of central fields, in which $U \propto \frac{1}{r}$, and force $\left(F = -\frac{dU}{dr}\right)$

accordingly varies as $\frac{1}{r^2}$. (Newton gravitational attraction, coulomb electrostatic interaction)

Let us first consider an attractive field, where $U = -\frac{\alpha}{r}$, $\alpha > 0$.

From eq.(3.11) $U_{eff} = -\frac{\alpha}{r} + \frac{M^2}{2mr^2}$

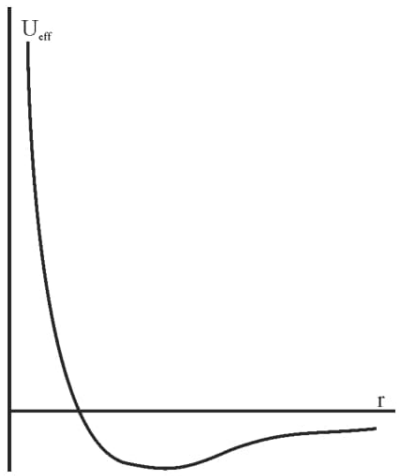


Figure 3.7

$r \to 0$, $U_{eff} \to +\infty$ $\quad \left\{ U_{eff} \to \left(-\alpha.\infty + \frac{M}{2m}.\infty^2 \right) \to +\infty \right\}$

and $r \to \infty$, $U_{eff} \to 0$ from negative values $\left\{ U_{eff} \to \left(-\alpha.0 + \frac{M}{2m}.0^2 \right) \to 0 \right\}$

$$\frac{dU}{dr} = \frac{\alpha}{r^2} - \frac{M^2}{mr^3} \quad \& \frac{d^2U}{dr^2} = -2\frac{\alpha}{r^3} + 3\frac{M^2}{mr^4}$$

For maxima - minima $\frac{dU}{dr} = 0$ *i.e.* $\frac{\alpha}{r^2} - \frac{M^2}{mr^3} = 0 \Rightarrow r = \frac{M^2}{m\alpha}$

At $r = \frac{M^2}{m\alpha}$ value of $\frac{d^2U}{dr^2}$ is given by

$$\frac{d^2U}{dr^2} = -2\frac{\alpha}{\left(\frac{M^2}{m\alpha}\right)^3} + 3\frac{M^2}{m\left(\frac{M^2}{m\alpha}\right)^4} = -2\frac{m^3\alpha^4}{M^6} + 3\frac{m^3\alpha^4}{M^6} = \frac{m^3\alpha^4}{M^6}$$

$$\frac{d^2U}{dr^2} > 0$$

So at $r = \frac{M^2}{m\alpha}$ it has minima. The value of U_{eff} is given by

$$U_{eff,\min} = -\frac{\alpha}{r} + \frac{M^2}{2mr^2} = -\frac{\alpha}{\left(\frac{M^2}{m\alpha}\right)} + \frac{M^2}{2m\left(\frac{M^2}{m\alpha}\right)^2} = -\frac{m\alpha^2}{M^2} + \frac{m\alpha^2}{2M^2}$$

$$U_{eff,\min} = -\frac{m\alpha^2}{2M^2} \tag{3.22}$$

It is seen from the figure, that the motion is finite for $E < 0$ and infinite for $E > 0$. The shape of the path is obtained from the formula(3.10)

$$\phi = \int \frac{Mdr/r^2}{\sqrt{\left\{2m\left[E - U(r)\right] - \frac{M^2}{r^2}\right.}} + \text{Constant}$$

$$\phi = \int \frac{M}{mr^2} \frac{dr}{\sqrt{\frac{2}{m}\left(E + \frac{\alpha}{r} - \frac{M^2}{2mr^2}\right)}} + \text{Constant} \quad \because U(r) = -\frac{\alpha}{r}$$

$$\phi = \int \frac{Mdr}{mr^2\sqrt{\frac{2}{m}\left\{E + \frac{\alpha}{r} - \frac{M^2}{2mr^2} - \frac{m\alpha^2}{2M^2} + \frac{m\alpha^2}{2M^2}\right\}}} + \text{Constant}$$

$$\phi = \int \frac{Mdr}{mr^2\sqrt{\frac{2}{m}\left\{\left(E + \frac{m\alpha^2}{2M^2}\right) + \frac{\alpha}{r} - \frac{M^2}{2mr^2} - \frac{m\alpha^2}{2M^2}\right\}}} + \text{Constant}$$

$$\phi = \int \frac{Mdr}{mr^2\sqrt{\frac{2}{m}\left\{\left(E + \frac{m\alpha^2}{2M^2}\right) - \frac{M^2}{2m}\left(\frac{1}{r^2} - \frac{2m\alpha}{M^2 r} + \frac{m^2\alpha^2}{M^4}\right)\right\}}} + \text{Constant}$$

$$\varphi = \int \frac{M}{mr^2}\sqrt{\frac{m}{2}}\frac{dr}{\left\{\left(E+\frac{\alpha^2 m}{2M^2}\right)-\frac{M^2}{2m}\left(\frac{1}{r}-\frac{\alpha m}{M^2}\right)^2\right\}^{\frac{1}{2}}} + \text{Constant} \qquad (3.23)$$

For $E+\frac{\alpha^2 m}{2M^2} > 0$, Let $A^2 = E+\frac{\alpha^2 m}{2M^2}$, $X = \frac{1}{r}-\frac{\alpha m}{M^2}$ or $dX = -\frac{dr}{r^2}$

Putting these values in eq.(3.23)

or $$\phi = \int \frac{M}{\sqrt{2m}}(-1)\frac{dX}{\sqrt{A^2-\frac{M^2}{2m}X^2}} + \text{Constant}$$

$$\phi = \int \frac{M}{\sqrt{2m}}\frac{(-dX)}{\frac{M}{\sqrt{2m}}\sqrt{\frac{2mA^2}{M^2}-X^2}} + \text{Constant}$$

$$\phi = \int \frac{(-dX)}{\sqrt{\left(\frac{\sqrt{2m}A}{M}\right)^2-X^2}} + \text{Constant}$$

Taking the origin of ϕ such that the constant is zero, we find

$$\phi = \cos^{-1}\left(\frac{X}{\frac{\sqrt{2m}A}{M}}\right) + \text{Constant}$$

$$\cos\phi = \frac{MX}{\sqrt{2m}A} \quad \text{or} \quad \frac{\sqrt{2m}A}{M}\cos\phi = X$$

Putting values of X and A, We get

$$\frac{\sqrt{2m}}{M}\sqrt{E+\frac{\alpha^2 m}{2M^2}}\,.\cos\phi = \frac{1}{r}-\frac{\alpha m}{M^2}$$

$$\Rightarrow \frac{\sqrt{2m}}{M}\sqrt{\frac{\alpha^2 m}{2M^2}\left(1+\frac{2M^2E}{m\alpha^2}\right)}.\cos\phi = \frac{1}{r}-\frac{\alpha m}{M^2}$$

$$\Rightarrow \frac{m\alpha}{M^2}\sqrt{\left(1+\frac{2M^2E}{m\alpha^2}\right)}.\cos\phi = \frac{1}{r}-\frac{\alpha m}{M^2}$$

$$\Rightarrow \frac{m\alpha}{M^2}\left(1+\sqrt{1+\frac{2M^2E}{m\alpha^2}}\cos\phi\right).=\frac{1}{r}$$

$$\Rightarrow \quad 1+\sqrt{1+\frac{2M^2E}{m\alpha^2}}\cos\phi=\left(\frac{M^2}{m\alpha}\right)\frac{1}{r}$$

or $$\frac{p}{r}=1+e\cos\varphi \tag{3.24}$$

where $p=\frac{M^2}{m\alpha}, e=\sqrt{1+\frac{2M^2E}{m\alpha^2}}$ (3.25)

This is the equation of conic section with one focus at the origin, $2p$ is called the latus rectum of the orbit and e the eccentricity.

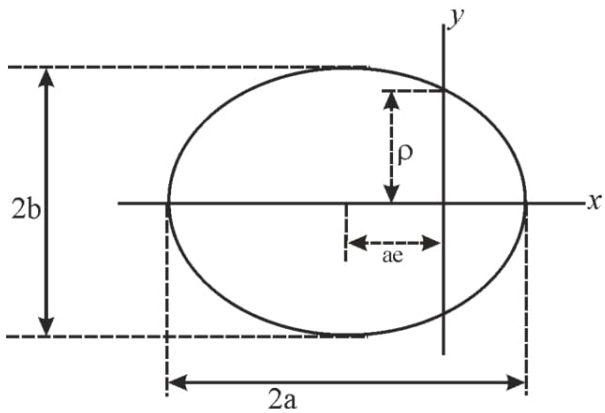


Figure 3.8

Our choice of the origin of ϕ is seen to be such that the point where $\phi=0$ is the point nearest to the origin (called the perihelion).

$$[\because \phi=0, \cos\phi=1, \frac{1}{r}=1+e=\text{maximum i.e. } r=r_{\min}]$$

In the equivalent problem of two particles interacting according to the law $U=-\frac{\alpha}{r}$***, the orbit of each particle is a conic section, with one focus at the centre of mass of the two particles***.

If energy E is negative i.e. $E<0$***, then*** $e<1$ $\left(\because e=\sqrt{1+\frac{2M^2E}{m\alpha^2}}\right)$ ***i.e. for*** $E<0$, $e<1$ ***the orbit is ellipse and the motion is finite.***

According to the formulae to analytical geometry, the major and minor semi-axes of the ellipse are:

Semi major axis $a = \dfrac{p}{1-e^2}$, Semi minor axis $b = \dfrac{p}{\sqrt{1-e^2}}$

Here $b = \dfrac{p}{\sqrt{1-e^2}} = \dfrac{p}{(1-e^2)}\sqrt{1-e^2} = a\sqrt{1-e^2}$

From eq(3.25)putting values of p and e in expressions of a and b

$$a = \frac{p}{1-e^2} = \frac{\left(\dfrac{M^2}{m\alpha}\right)}{1-\left(1+\dfrac{2M^2E}{m\alpha^2}\right)} = -\frac{\alpha}{2E} = \frac{\alpha}{2|E|} \qquad \{\because E = -|E|$$

$$b = \frac{p}{\sqrt{1-e^2}} = \frac{\left(\dfrac{M^2}{m\alpha}\right)}{\sqrt{1-\left(1+\dfrac{2M^2E}{m\alpha^2}\right)}} = \frac{M}{\sqrt{-2mE}} = \frac{M}{\sqrt{2m|E|}}$$

Thus $a = \dfrac{p}{1-e^2} = \dfrac{\alpha}{2|E|}$, $b = \dfrac{p}{\sqrt{1-e^2}} = a\sqrt{1-e^2} = \dfrac{M}{\sqrt{2m|E|}}$ (3.26)

Energy E=T+U ,when kinetic energy is zero, then the least possible value of the energy is

$E = 0 + U_{eff,\min}$

Using eq.(3.22) , we have $\mathrm{E} = -\dfrac{m\alpha^2}{2M^2}$

and then $e = \sqrt{1+\dfrac{2M^2E}{m\alpha^2}} = 0$, i.e. ***the ellipse(e<1) becomes a circle(e = 0).***

It may be noted that the major axis $\left(a = \dfrac{\alpha}{2|E|}\right)$ of the ellipse depends only on the energy E of the particle, and not on its angular momentum M.

By eq.(3.24)

$$\boxed{\frac{p}{1+e\cos\varphi}=r}$$

The least and greatest distances from the centre of the field (the focus of the ellipse) are

Using(3.26),we have

$$\text{Here}\begin{cases} r_{\min}=\dfrac{p}{1+e}=\dfrac{p}{(1+e)(1-e)}(1-e)=\dfrac{p}{1-e^2}(1-e)=a(1-e) \\ r_{\max}=\dfrac{p}{1-e}=\dfrac{p}{(1-e)(1+e)}(1+e)=\dfrac{p}{1-e^2}(1+e)=a(1+e) \end{cases}$$

$$\text{Thus}\quad \boxed{r_{\min}=\frac{p}{1+e}=a(1-e)\ ,\ r_{\max}=\frac{p}{1-e}=a(1+e)} \qquad (3.27)$$

The period T of revolution in an elliptical orbit is conveniently found by using the law of conservation of angular momentum in the form of the area integral.

By eq.(3.6)

$$\therefore \qquad df=\frac{1}{2}r.rd\theta$$

$$\text{Or}\quad \frac{df}{dt}=\frac{1}{2}r^2\frac{d\theta}{dt}$$

$$2\frac{df}{dt}=\frac{M}{m} \qquad \therefore \text{By eq.(3.6)} \quad M=2m\frac{df}{dt}, M=\text{ Angular Momentum}$$

$$\text{or} \qquad df=\frac{M}{2m}dt$$

$$\text{or} \qquad f=\frac{M}{2m}.T \qquad (f=\text{area of ellipse},\ T=\text{period of revolution})$$

$$\therefore \qquad T=\frac{2m}{M}.\pi ab \qquad (\because f=\pi ab=\text{area of ellipse})$$

$$T=\frac{2m}{M}\pi a.\frac{M}{\sqrt{2m|E|}} \qquad \because \text{By eq. (3.26)} \quad b=\frac{M}{\sqrt{2m|E|}}$$

$$=\frac{2m\pi a}{\sqrt{2m\dfrac{\alpha}{2a}}} \qquad \because \text{By eq. (3.26)} \quad a=\frac{\alpha}{2|E|}$$

$$T = \left(\frac{4m^2\pi^2}{m\alpha}\right)^{\frac{1}{2}} a^{3/2} = \sqrt{\frac{m}{\alpha}}.2\pi\, a^{3/2} \quad or \boxed{T \propto a^{3/2}}$$

Using eq.(3.26)

$$T = \pi\alpha\sqrt{\frac{m}{2|E|^3}}$$

i.e. period depends only on the energy of the particle.

For $E \geq 0$ ***particle is not in bound state i.e. the motion is infinite. If*** $E > 0$ ***, the eccentricity*** $e = \sqrt{1 + \frac{2M^2E}{m\alpha^2}} > 1$***, i.e. the path is hyperbola*** with origin as internal focus.

The distance of the perihelion from the focus is

By eq.(3.27) $r_{\min} = \frac{p}{e+1} = a(e-1)$

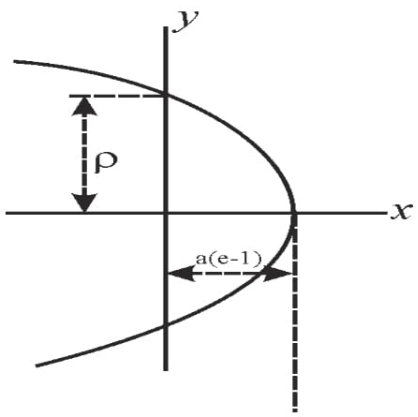


Figure 3.9

Where $a = \frac{p}{e^2-1} = \frac{\alpha}{2|E|}$ is the "semi axis" of the hyperbola

If $E = 0$, the eccentricity $e = \sqrt{1 + \frac{2M^2E}{m\alpha^2}} = 1$,then $r_{\min} = \frac{p}{1+e} = \frac{1}{2}p$. This case occur if the particle starts from rest at infinity.

To conclude this section , we shall show that there is an integral of the motion

which exists only in fields $U = \frac{\alpha}{r}$ (with either sign of α). It is easy to verify by direct calculation that the quantity.

$$\vec{A} \equiv \vec{v} \times \vec{M} + \alpha \frac{\vec{r}}{r} \text{ is constant} \tag{3.28}$$

To verify this, we differentiate $\vec{A}$ w.r.t time:

$$\dot{\vec{A}} = \dot{\vec{v}} \times \vec{M} + \vec{v} \times \dot{\vec{M}} + \alpha \frac{\dot{\vec{r}}}{r} + \alpha \vec{r}\left(-\frac{1}{r^2}\right)\dot{r}$$

$$\left\{ \because \vec{M} = \text{constant} \Rightarrow \dot{\vec{M}} = 0 \text{ and } \vec{v} = \dot{\vec{r}} \right.$$

$$\therefore \dot{\vec{A}} = \dot{\vec{v}} \times \vec{M} + \alpha \frac{\vec{v}}{r} + \alpha \vec{r}\left(-\frac{1}{r^3}\right) r\dot{r}$$

$$\begin{cases} \because r^2 = \vec{r}^2 \Rightarrow \dfrac{dr^2}{dt} = \dfrac{d\vec{r}^2}{dt} \\ \Rightarrow 2r\dfrac{dr}{dt} = 2\vec{r}.\dfrac{d\vec{r}}{dt} \Rightarrow r\dot{r} = \vec{r}.\dot{\vec{r}} \Rightarrow r\dot{r} = \vec{r}.\vec{v} \end{cases}$$

$$\therefore \dot{\vec{A}} = \dot{\vec{v}} \times \vec{M} + \alpha \frac{\vec{v}}{r} + \alpha \vec{r}\left(-\frac{1}{r^3}\right)\left(r.\dot{\vec{v}}\right)$$

$$= \dot{\vec{v}} \times \left(\vec{r} \times m\vec{v}\right) + \frac{\alpha \vec{v}}{r} - \frac{\alpha \vec{r}}{r^3}\left(\vec{v}.\vec{r}\right)$$

$$\left\{ \because \vec{A} \times \left(\vec{B} \times \vec{C}\right) = \vec{B}\left(\vec{A}.\vec{C}\right) - \vec{C}\left(\vec{A}.\vec{B}\right) \right\}$$

$$\dot{\vec{A}} = \vec{r}\left(\dot{\vec{v}}.m\vec{v}\right) - m\vec{v}\left(\dot{\vec{v}}.\vec{r}\right) + \frac{\alpha \vec{v}}{r} - \frac{\alpha \vec{r}}{r^3}\left(\vec{v}.\vec{r}\right)$$

$$\dot{\vec{A}} = \vec{r}\left(\vec{v}.m\dot{\vec{v}}\right) - \vec{v}\left(\vec{r}.m\dot{\vec{v}}\right) + \frac{\alpha \vec{v}}{r} - \frac{\alpha \vec{r}}{r^3}\left(\vec{v}.\vec{r}\right) = 0 \tag{3.29}$$

We know that force $\vec{F} = \frac{d\left(m\vec{v}\right)}{dt} = m\dot{\vec{v}}$ but $\vec{F} = -\frac{dU}{dr}\hat{r}$

$$\text{Thus } m\dot{\vec{v}} = -\frac{dU}{dr}\hat{r} \Rightarrow m\dot{\vec{v}} = -\frac{d}{dr}\left(\frac{\alpha}{r}\right)\hat{r} \Rightarrow m\dot{\vec{v}} = \frac{\alpha}{r^2}\hat{r}$$

$$\Rightarrow m\dot{\vec{v}} = \frac{\alpha}{r^2}\frac{\vec{r}}{r} \qquad \Rightarrow \qquad m\dot{\vec{v}} = \frac{\alpha \vec{r}}{r^3}$$

Putting this value in eq.(3.29)

$$\dot{\vec{A}} = \vec{r}\left(\vec{v}.\frac{\alpha\vec{r}}{r^3}\right) - \vec{v}\left(\vec{r}.\frac{\alpha\vec{r}}{r^3}\right) + \frac{\alpha\vec{v}}{r} - \frac{\alpha\vec{r}}{r^3}(\vec{v}.\vec{r})$$

$$\dot{\vec{A}} = \frac{\alpha\vec{r}}{r^3}(\vec{v}.\vec{r}) - \alpha\vec{v}\left(\frac{\vec{r}.\vec{r}}{r^3}\right) + \frac{\alpha\vec{v}}{r} - \frac{\alpha\vec{r}}{r^3}(\vec{v}.\vec{r})$$

$$\dot{\vec{A}} = -\alpha\vec{v}\left(\frac{\vec{r}.\vec{r}}{r^3}\right) + \frac{\alpha\vec{v}}{r}$$

$$\dot{\vec{A}} = 0 \qquad \left\{\because \frac{\vec{r}.\vec{r}}{r^3} = \frac{r^2}{r^3} = \frac{1}{r}\right\}$$

We find that this expression vanishes.

The direction of the conserved vector is along the major axis from the focus to the perihelion, and its magnitude is αe:

$$\vec{A} = \vec{v} \times \vec{M} + \alpha\frac{\vec{r}}{r}$$

$$\vec{A} = \vec{v} \times (\vec{r} \times m\vec{v}) + \alpha\frac{\vec{r}}{r}$$

$$\vec{A} = m[\vec{r}(\vec{v}.\vec{v}) - \vec{v}(\vec{r}.\vec{v})] + \alpha\frac{\vec{r}}{r}$$

We consider its value at perihelion(closest distance)

$$\vec{A} = m\{\vec{r}\,v^2 - \vec{v}(\vec{v}.\vec{r})\} + \alpha\frac{\vec{r}}{r}$$

$$= mv^2\vec{r} + \alpha\frac{\vec{r}}{r} \qquad \{\because \vec{v} \perp \vec{r} = 0 \quad \therefore \vec{v}.\vec{r} = 0 \text{ at perihelion}$$

$$|\vec{A}| = \left|mv^2 + \frac{\alpha}{r}\right||\vec{r}| = \left|mv^2 + \frac{\alpha}{r}\right|r$$

$$|\vec{A}| = |mv^2 r + \alpha|$$

Using eq.(3.27) at perihelion $r_{\min} = r = a(e-1)$

Using this value in

$$\therefore |\vec{A}| = |mv^2[a(e-1)] + \alpha| \qquad (3.30)$$

$$\because E = T + U \ , U = \frac{\alpha}{r} \ \Rightarrow \ \mathrm{E} = \frac{1}{2}mv^2 + \frac{\alpha}{r} \quad \text{or} \quad mv^2 = 2E - \frac{2\alpha}{r}$$

Using this value of mv^2 in eq.(3.30)

$$\left|\vec{A}\right| = \left|\left(2E - \frac{2\alpha}{r}\right)a(e-1) + \alpha\right|$$

$$\left|\vec{A}\right| = \left|\left(2E - \frac{2\alpha}{a(e-1)}\right)a(e-1) + \alpha\right|$$

$\because$ At perihelion $\quad r = a(e-1)$

$$\left|\vec{A}\right| = \left|\left(2Ea(e-1) - 2\alpha\right) + \alpha\right|$$

$$\left|\vec{A}\right| = \left|2Ea(e-1) - \alpha\right|$$

$$\left|\vec{A}\right| = \left|-\alpha\,(e-1) - \alpha\right|$$

$$\left\{\begin{array}{l} \because \text{ By eq.(3.26)} \quad a = \dfrac{\alpha}{2|E|} \Rightarrow 2a|E| = \alpha \\ \Rightarrow 2a(-E) = \alpha \quad \text{For bound state} \ \ \mathrm{E} = -|\mathrm{E}| \end{array}\right\}$$

$$\left|\vec{A}\right| = \left|-\alpha e + \alpha - \alpha\right| = \left|-\alpha e\right|$$

$$\left|\vec{A}\right| = \left|\alpha e\right|$$

Similarly we can prove that $\vec{A} \equiv \vec{v} \times \vec{M} - \alpha\dfrac{\vec{r}}{r}$ is conserved for $U = -\dfrac{\alpha}{r}$ and The direction of the conserved vector is along the major axis from the focus to the perihelion, and its magnitude is $\alpha\, e$:

The coordinate of the particle as functions of time in the orbit may be found by the general formula

Using eq.(3.7)

$$E = \frac{1}{2}m\dot{r}^2 + \frac{M^2}{2mr^2} + U(r)$$

Using eq.(3.11)

$$E = \frac{1}{2}m\dot{r}^2 + U_{eff} \quad \text{where } U_{eff} = \frac{M^2}{2mr^2} + U(r) = \frac{M^2}{2mr^2} + \frac{-\alpha}{r} \ , U(r) = -\frac{\alpha}{r}$$

$$\frac{2}{m}\left(E-U_{eff}\right)=\dot{r}^2$$

$$dt=\frac{dr}{\sqrt{\frac{2}{m}\left(E-U_{eff}\right)}}$$

$$t=\int\frac{dr}{\sqrt{\frac{2}{m}\left(E+\frac{\alpha}{r}-\frac{M^2}{2mr^2}\right)}}$$

Putting $E=-|E|$

$$t=\int\frac{dr}{\sqrt{\frac{2}{m}\left(-|E|+\frac{\alpha}{r}-\frac{M^2}{2mr^2}\right)}}$$

$$t=\int\frac{dr}{\sqrt{\frac{2|E|}{m}\left(-|E|+\frac{\alpha r}{|E|}-\frac{M^2}{2m|E|}\right)}}$$

$$=\sqrt{\frac{m}{2|E|}}\int\frac{r\,dr}{\sqrt{\left[-r^2+\frac{\alpha\, r}{|E|}-\frac{M^2}{2m|E|}\right]}}$$

$$\left\{\text{By eq.(3.26)}\quad a=\frac{\alpha}{2|E|}\Rightarrow 2a=\frac{\alpha}{|E|},b=\frac{p}{\sqrt{1-e^2}}=\frac{M}{\sqrt{2m|E|}}\right\}$$

$$\therefore t=\sqrt{\frac{m2a}{2\alpha}}\int\frac{r\,dr}{\left[-r^2+2a\,r-\frac{p^2}{1-e^2}\right]^{\frac{1}{2}}}$$

$$\because a=\frac{p}{1-e^2}\ \Rightarrow a\left(1-e^2\right)=p\ \text{ Using the value of p, We have}$$

$$t=\sqrt{\frac{ma}{\alpha}}\int\frac{r\,dr}{\left[-a^2\left(1-e^2\right)-r^2+2ar\right]^{\frac{1}{2}}}$$

$$t = \sqrt{\frac{ma}{\alpha}} \int \frac{r\,dr}{\sqrt{a^2e^2 - (r-a)^2}}$$

Let $r - a = -ae\cos\xi$ (3.31)

$\Rightarrow dr = ae\sin\xi d\xi$ Putting these values in above expression

$$\therefore t = \sqrt{\frac{ma}{\alpha}} \int \frac{a(1-e\cos\xi).ae\sin\xi\, d\xi}{\sqrt{a^2e^2 - a^2e^2\cos^2\xi}}$$

$$\therefore t = \sqrt{\frac{ma^3}{\alpha}} \int (1-e\cos\xi)d\xi$$

$$= \sqrt{\frac{ma^3}{\alpha}} .(\xi - e\sin\xi) + \text{ Constant} \qquad (3.32)$$

If time is measured in such a way that the constant is zero(we assume $\xi = 0$ at $t = 0$ then by eq.(3.32)

$$0 = \sqrt{\frac{ma^3}{\alpha}} .(0 - e\sin 0) + \text{ Constant} \Rightarrow 0 = \text{Constant})$$

we have the following parametric dependence on r and t :

By eq.(3.31) and (3.32)

$$, r = a(1-e\cos\xi) , t = \sqrt{\frac{ma^3}{\alpha}}(\xi - e\sin\xi) \qquad (3.33)$$

$\{ \because r - a = -ae\cos\xi \}$

the particle being at perihelion at $t = 0$

$\{\because At\ t = 0, \xi = 0 \Rightarrow r = a(1-e\cos 0) \Rightarrow r = a(1-e) Perihelion\}$.

The Cartesian coordinates

$x = r\cos\phi$, $y = r\sin\phi$ (the x and y -axis

being respectively parallel to the major and minor axes of the ellipse) can be expressed in thus of the parameter ξ.

$$\because \frac{p}{r} = 1 + e\cos\phi \Rightarrow p = r + re\cos\phi$$

$$\Rightarrow p = r + ex \ \{ \because x = r\cos\phi \ \}$$

$$\Rightarrow ex = p - r$$

Using eq.(3.33)

$$ex = a\left(1-e^2\right) - a(1 - e\cos\xi) \quad \{p = a\left(1-e^2\right)\}$$

$$= a - ae^2 - a + ae\cos\xi$$

$$ex = ae(\cos\xi - e)$$

$$x = a(\cos\xi - e)$$

$$(x + ae) = a\cos\xi \qquad (3.34)$$

$$y = \sqrt{r^2 - x^2}$$

Using eq.(3.33) and (3.34)

$$y = \sqrt{\{a(1-e\cos\xi)\}^2 - \{a(\cos\xi - e)\}^2}$$

$$= \sqrt{a^2\left(1 + e^2\cos^2\xi - 2e\cos\xi\right) - a^2\left(\cos^2\xi + e^2 - 2e\cos\xi\right)}$$

$$= a\sqrt{1 - \cos^2\xi - e^2 + e^2\cos^2\xi}$$

$$= a\sqrt{\sin^2\xi - e^2\sin^2\xi}$$

$$y = a\sin\xi\sqrt{1-e^2}$$

$$y = b\sin\xi \qquad \left\{\because \text{By eq.(3.26)} \quad b = a\sqrt{1-e^2}\right\}$$

By eq.(3.34) we have $(x + ae) = a\cos\xi, y = b\sin\xi$

represents the parametric form of ellipse

$\left\{\frac{(x+ae)^2}{a^2} + \frac{y^2}{b^2} = 1\right.$ is equation of ellipse . It is obvious that a complete passage round the ellipse corresponds to an increase of ξ from 0 to 2π .

3.7 Self Learning Exercise-II

Section A:Very Short Answer Type Questions

Q.1 Kepler's second law follows from

(a) Law of conservation of Energy

(b) Law of Conservation of momentum

(c) Law of conservation of Angular momentum.

Q.2 What is centrifugal potential energy of a particle in any central field?

Section B: Short Answer Type Questions

Q.3 In the Kepler's problem, the trajectory of a particle is given by

$$\frac{p}{r} = 1 + e\cos\phi$$

Express p and e in terms of energy E and angular momentum M.

3.8 Summary

In this chapter we have discussed the problem of two bodies moving under the influence of a mutual central force interaction by using Lagrangian formulation. We have reduced the two body problem to that of an equivalent one-body problem of mass $m = \frac{m_1 m_2}{m_1 + m_2}$.

We have also found the trajectory of a particle in the field $U = -\frac{\alpha}{r}$. The trajectory is found to be $\frac{p}{r} = 1 + e\cos\phi$, where p and the eccentricity e have been expressed in terms of energy E and angular momentum M. In the Kepler's problem we have also verified that apart from the two integrals of motion viz-E and $\vec{M}$ there is an additional integral of motion defined by conserved vector $\vec{A} = \vec{v} \times \vec{M} + \alpha \frac{\vec{r}}{r}$, which is along the major axis from the focus to the perihelion and its magnitude is αe.

3.9 Glossary

Monotonically: quantity varying in such a way that it either never decreases or never increases.

Eccentricity: A measure of the extent of deviation from circularity

3.10 Answers to Self Learning Exercises

Answer to Self Learning Exercise-I

Ans. 4: Turning points are given by the equation

$$E = U(x)$$

$= \frac{1}{2}kx^2$, therefore $x = \pm\sqrt{\frac{2E}{k}}$

Ans. 5: $L = \frac{1}{2}m_1\dot{\vec{r}}_1^2 + \frac{1}{2}m_2\dot{\vec{r}}_2^2 - U(|\vec{r}_1 - \vec{r}_2|)$

Ans. 7: $\vec{r}_1 = \frac{m_2\vec{r}}{m_1 + m_2}, \vec{r}_2 = -\frac{m_1\vec{r}}{m_1 + m_2}$

Answer to Self Learning Exercise-II

Ans. 1: (c)

Ans. 2: $U = \frac{M^2}{2mr^2}$,where M is angular momentum of the particle, m is reduced mass. It is always positive. It tends to infinite value as $r \to 0$.

3.11 Exercise

Section A : Very Short Answer Type Questions

Q. 1 What are the turning points of the motion.

Q. 2 Write the Lagrangian of a particle in a potential field $U = U(x)$.

Q. 3 Write the equation of motion of a particle in this field.

Q. 4 What is the condition for the path to be closed?

Q. 5 Prove that angular momentum of a particles satisfies $M = 2m\dot{f}$ where $\dot{f}$ is the sectorial velocity.

Q. 6 What is a Cyclic coordinate.

Section B: Short Answer Type Questions

Q. 7 Show that the quantity $\vec{A} \equiv \vec{v} \times \vec{M} + \alpha\frac{\vec{r}}{r}$ is an integral of the motion which exists only in fields $U = \frac{\alpha}{r}$ (with either sign of α)

Q. 8 Derive the condition for the 'fall' of a particle to the centre of the field $U = U(r)$.

Q. 9 Derive an expression for the time period T of revolution in an elliptical orbit using the law of conservation of angular momentum in the form of the area integral.

Q. 10 Reduce the problem of motion of two interacting particles to that of the motion of one particle in a given external field $U = U(r)$.

Q. 11 Discuss the condition for the 'fall' of a particle to the centre of the field.

Section C : Long Answer Type Questions

Q. 12 Find the Trajectory of a particle in the field $U = -\frac{\alpha}{r}$ (Kepler's Problem). What is Runge-Lenz's vector. Show that it is conserved.

Q. 13 Integrate equations of motion for a particle in central field $U = -\frac{\alpha}{r^2}(\alpha > 0)$.

Q. 14 Determine the period of oscillations of a simple pendulum as a function of the amplitude of oscillations.

Q. 15 Derive an expression for the orbit of a particle in an attractive field $U = -\frac{\alpha}{r}$. Show that the orbit is given by

$$\frac{p}{r} = 1 + e\cos\phi .$$

Derive expression for p and e in terms of E and M.

What is the shape of the orbit if (a) E < 0 (b) E = 0 (c) E > 0.

Q. 16 Show that the motion of a particle in a Central field satisfies the following facts

(i) Angular momentum of the particle about the centre is conserved.

(ii) The path of the particle is in a plane perpendicular to $\overline{M}$.

(iii) The radial motion of the particle is a one dimensional motion in an effective field.

$$U = U(r) + \frac{M^2}{2mr^2}$$

(iv) Find the general equation in $r - \phi$ coordinate system.

3.12 Answers to Exercise

Ans. 2: $L = \frac{1}{2}m\dot{x}^2 - U(x)$

Ans. 3: $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}$

Or $m\ddot{x} = -\frac{\partial U}{\partial x}$

Ans. 4: $\Delta\phi = 2\pi\frac{m}{n}$

Where m and n are integers.

Ans. 7: For answer see the text.

Ans. 8: $\left[r^2U(r)\right]_{\lim r\to 0} < -\frac{M^2}{2m}, i.e.$

$U(r)$ must tend to $-\infty$ either as $-\frac{\alpha}{r^2}$ with $\alpha > \frac{M^2}{2m}$

Or proportionally to $-\frac{1}{r^n}$ with $n > 2$

Ans. 9: Sectorial area swept by the radius vector of the planet is

$$df = \frac{1}{2}r.rd\theta$$

or $2\frac{df}{dt} = \frac{M}{m}$

Integrating, we get $T = \frac{2m}{M}\pi ab$

Using $b = \frac{M}{\sqrt{2m|E|}}$, we finally get $T = \pi \times \sqrt{\frac{m}{2|E|^3}}$

i.e. period depends only on the energy of the particle.

Ans. 10: Define $\vec{r} = \vec{r_1} - \vec{r_2}$

and choose origin at the centre of mass, i.e.

$m_1\vec{r_1} + m_2\vec{r_2} = \vec{0}$, Solving for $\vec{r_1}$ and $\vec{r_2}$ gives

$$\vec{r_1} = \frac{m_2}{m_1 + m_2}\vec{r}, \vec{r_2} = -\frac{m_1}{m_1 + m_2}\vec{r}$$

So the Lagrangian of two interacting particles finally is found to be

$$L = \frac{1}{2}m\dot{\vec{r}}^2 - U(\vec{r}) \text{ Where } m = \frac{m_1 m_2}{m_1 + m_2}$$

References and Suggested Readings

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2. Gupta ,Kumar &Sharma ,Classical Mechanics, Pragati Prakashan Meerut , 1998

3. Goldstein, Poole &Saiko, Classical Mechanics,Pearson Education 2002

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UNIT- 4
Collisions between Particles

Structure of the Unit

4.0 Objectives

4.1 Introduction

4.2 Disintegration of Particles

4.3 Elastic Collisions

4.4 Rutherford's Formula

4.5 Self Learning Exercise-I

4.6 Summary

4.7 Glossary

4.8 Answers to Self Learning Exercise

4.9 Exercise

4.10 Answers to Exercise

References and Suggested Readings

4.0 Objectives

In this chapter we shall obtain important results concerning various mechanical processes e.g. scattering of particles, spontaneous disintegration of a particle by making use of the laws of conservation of momentum, energy alone.

4.1 Introduction

We shall study collisions between two particles in a centre of mass frame in which the centre of mass of the two particles is at rest. We shall find the relationship between the laboratory frame (L-frame) and C.M frame .We shall introduce an important concept of collision cross-section and calculate the scattering cross section for "Rutherford scattering "

4.2 Disintegration of Particles

In many cases the laws of conservation of momentum and energy alone can

be used to obtain important results concerning the properties of various mechanical processes. Let us consider a "spontaneous" disintegration of a particle into two "constituent parts", i.e. into two other particles which move independently after the disintegration". This process is most simply described in ***a frame of reference in which the particle is at rest before the disintegration i.e. in centre of mass frame***.

In centre of mass (C.M.) frame momentum of the original particle is zero. After disintegration particles move with momenta $\vec{p}_{1C}$ and $\vec{p}_{2C}$, by momentum conservation $0 = \vec{p}_{1C} + \vec{p}_{2C}$ i.e. $\vec{p}_{1C} = -\vec{p}_{2C}$

Let $\left|\vec{p}_{1C}\right| = \left|\vec{p}_{2C}\right| = p_0$

In C.M. frame kinetic energies of the first and second particle are $\frac{p_0^2}{2m_1}$ and $\frac{p_0^2}{2m_2}$ respectively and internal energies are E_{1i} and E_{2i} respectively. Where m_1 and m_2 represent the masses of the first and second particle respectively.

After disintegration energy of the first particle is $E_{1i} + K.E_1$ *i.e.* $E_{1i} + \frac{p_0^2}{2m_1}$

After disintegration energy of the second particle is $E_{2i} + K.E_2$ *i.e.* $E_{2i} + \frac{p_0^2}{2m_2}$

By energy conservation

$$E_i = E_{1i} + \frac{p_0^2}{2m_1} + E_{2i} + \frac{p_0^2}{2m_2}$$

$$\therefore \text{Disintegration energy } \varepsilon = E_i - \left(E_{1i} + E_{2i}\right) = \frac{p_0^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right) = \frac{p_0^2}{2m}$$

Where $\boxed{\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2} \Rightarrow m = \frac{m_1 m_2}{m_1 + m_2} = \text{reduced mass of the system}}$ ....(4.1)

Let us now change to a frame of reference in which the primary (original) particle moves with velocity $\vec{V}$ before the splitting (This Laboratory system is known as L-system). As initially there is only one particle so centre of mass of the system is the particle itself. Therefore velocity of centre of mass is also equal to $\vec{V}$ .As there is no external force on the system, so C.M. of the system moves with same velocity $\vec{V}$ after disintegration. Let after disintegration $\vec{v}_{1L}$ and $\vec{v}_{1C}$ be the

velocities of the first particle in the L and C.M. system respectively. Here centre of mass frame of reference is known as C.M. system or C system.

Velocity of particle w.r.t. L frame = Velocity of C.M. w.r.t. L frame + Velocity of particle w.r.t. C.M. frame

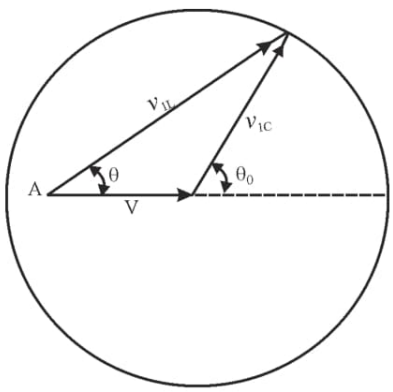
$$\Rightarrow \vec{v}_{1L} = \vec{V} + \vec{v}_{1C} \qquad (4.2)$$

$$\text{or } \vec{v}_{1L} - \vec{V} = \vec{v}_{1C}$$

$$\text{or } v_{1L}^2 + V^2 - 2v_{1L}V\cos\theta_{1L} = v_{1C}^2 \quad ,$$

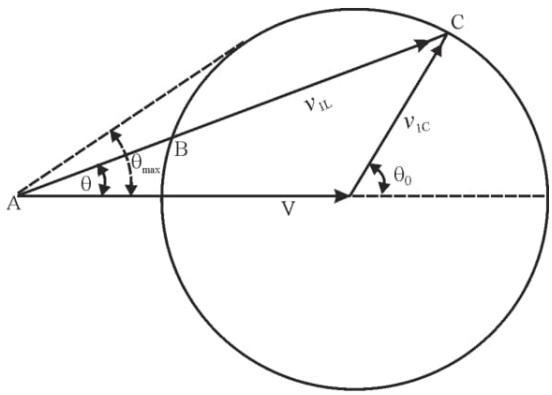
where θ_{1L} is the angle between $\vec{v}_{1L}$ and $\vec{V}$ i.e. θ_{1L} is the angle at which this particle moves relative to the direction of the velocity $\vec{V}$ in L frame.

We can draw vector diagram using eq.(4.2)



(a)V<v_{1C}

Figure 4.1



(*b*)V > v_{1C}

Figure 4.2

In CM frame the first particle can move in any direction i.e. $\vec{v}_{1C}$ can take orientation in any direction. Thus $\vec{v}_{1C}$ can rotate from 0 to 2π in diagrams (4.1) & (4.2)

Case(i) From diagram(4.1) it is obvious that if $V < v_{1C}$, θ_{1L} can have any value from 0 to 2π. This means $\vec{v}_{1L}$ can make any angle with $\vec{V}$ i.e. in L frame the first particle can move backwards.

Here $-\frac{\pi}{2} < \theta_{1L} < \frac{\pi}{2}$ represents the forward motion . We can say that if θ_{1L} lies in 1^{st} or 4^{th} quadrant, then motion of the particle will be in forward direction .

Here $\frac{\pi}{2} < \theta_{1L} < \frac{3\pi}{2}$ represents the backward motion . We can say that if θ_{1L} lies in 2^{nd} or 3^{rd} quadrant, then motion of the particle will be in backward direction .

Case(ii) If $V > v_{1C}$, From diagram(4.2) it is obvious that if θ_{1L} cannot exceed θ_{max} where $\sin\theta_{\max} = \frac{v_{1C}}{V} < 1$ i.e. magnitude of θ_{1L} is always less $\frac{\pi}{2}$,therefore the particle can move only forwards.

The relation between the angles θ_{1L} and θ_{1C} in the L and C system is evidently.

$$\tan\theta_{1L} = \frac{v_{1C}\sin\theta_{1C}}{V + v_{1C}\cos\theta_{1C}}$$

We can find the θ_{1C} in terms of θ_{1L}. Squaring the above expression

$$\tan^2\theta_{1L} = \frac{v_{1C}^2\sin^2\theta_{1C}}{V^2 + v_{1C}^2\cos^2\theta_{1C} + 2Vv_{1C}\cos\theta_{1C}}$$

$$\Rightarrow \tan^2\theta_{1L} = \frac{v_{1C}^2(1-\cos^2\theta_{1C})}{V^2 + v_{1C}^2\cos^2\theta_{1C} + 2Vv_{1C}\cos\theta_{1C}}$$

$$\Rightarrow V^2 + v_{1C}^2\cos^2\theta_{1C} + 2Vv_{1C}\cos\theta_{1C} = v_{1C}^2(1-\cos^2\theta_{1C})\cot^2\theta_{1L}$$

$$\Rightarrow \cos^2\theta_{1C}\left[v_{1C}^2(1+\cot^2\theta_{1L})\right] + \cos\theta_{1C}(2Vv_{1C}) + \left(V^2 - v_{1C}^2\cot^2\theta_{1L}\right) = 0$$

$$\Rightarrow \cos^2\theta_{1C}\left(v_{1C}^2\,\mathrm{cosec}^2\theta_{1L}\right) + \cos\theta_{1C}(2Vv_{1C}) + \left(V^2 - v_{1C}^2\cot^2\theta_{1L}\right) = 0$$

$$\Rightarrow \cos\theta_{1C} = \frac{-(2Vv_{1C}) \pm \sqrt{(2Vv_{1C})^2 - 4\left(v_{1C}^2\,\mathrm{cosec}^2\theta_{1L}\right)\left(V^2 - v_{1C}^2\cot^2\theta_{1L}\right)}}{2\left(v_{1C}^2\,\mathrm{cosec}^2\theta_{1L}\right)}$$

$$\Rightarrow \cos\theta_{1C} = \frac{-(V) \pm \sqrt{(V)^2 - \left(V^2\,\mathrm{cosec}^2\theta_{1L} - v_{1C}^2\cot^2\theta_{1L}\,\mathrm{cosec}^2\theta_{1L}\right)}}{\left(v_{1C}\,\mathrm{cosec}^2\theta_{1L}\right)}$$

$$\Rightarrow \cos\theta_{1C} = -\frac{V}{v_0}\sin^2\theta_{1L} \pm \sin^2\theta_{1L}\frac{\sqrt{V^2 - V^2\,\mathrm{cosec}^2\theta_{1L} + v_0^2\cot^2\theta_{1L}\,\mathrm{cosec}^2\theta_{1L}}}{(v_0)}$$

$$\Rightarrow \cos\theta_{1C} = -\frac{V}{v_{1C}}\sin^2\theta_{1L} \pm \sin^2\theta_{1L}\sqrt{\frac{V^2}{v_{1C}^2}\left(\frac{\sin^2\theta_{1L}-1}{\sin^2\theta_{1L}}\right) + \frac{\cos^2\theta_{1L}}{\sin^4\theta_{1L}}}$$

$$\Rightarrow \cos\theta_{1C} = -\frac{V}{v_{1C}}\sin^2\theta_{1L} \pm \sqrt{\frac{V^2}{v_{1C}^2}\sin^2\theta_{1L}(-\cos^2\theta_{1L}) + \cos^2\theta_{1L}}$$

$$\therefore \cos\theta_{1C} = -\frac{V}{v_{1C}}\sin^2\theta_{1L} \pm \cos\theta_{1L}\sqrt{\left(1 - \frac{V^2}{v_{1C}^2}\sin^2\theta_{1L}\right)}$$

➢ In the physical applications we are usually concerned with the disintegration of not one but many similar particles and this raises the problem of

the distribution of the resulting particles in direction, energy etc. We shall assume that the primary particles are randomly oriented in space, i.e. isotropically on average.

➢ In the C system, this problem is very easily solved; every resulting particle (of a given kind) has the same energy, and their direction of motion are isotropically distributed.

After disintegration θ_0 is the angle at which this particle moves relative to the direction of the velocity $\vec{V}$ in C frame.

The fractions of particles entering a solid angle element $d\Omega$ is proportional to $d\Omega$ i.e. equal to

$$\boxed{\frac{d\Omega}{4\pi} = \frac{\left(\frac{dA}{R^2}\right)}{4\pi} = \frac{dA}{4\pi R^2} = \frac{(2\pi R\sin\theta_0)(Rd\theta_0)}{4\pi R^2} = \frac{1}{2}\sin\theta_0 d\theta_0} \qquad (4.3)$$

The corresponding distribution in the L-system are obtained by an appropriate transformation. For example, let us calculate the kinetic energy distribution in L-system:

Using eq.(4.2)

$$\vec{v} = \vec{v}_0 + \vec{V} \qquad (4.4)$$

Where $\vec{v}$ is the velocity of the particle after disintegration in L frame and $\vec{v}_0$ is the velocity of the particle after disintegration in C frame.

From diagram (4.1) θ_0 is the angle between $\vec{v}_0$ and $\vec{V}$

$$\Rightarrow v^2 = v_0^2 + V^2 + 2v_0 V\cos\theta_0$$

Differentiating both sides

$$d\left(v^2\right) = d\left(2v_0 V\cos\theta_0\right)$$

$$\Rightarrow d\left(v^2\right) = 2v_0 V d(\cos\theta_0)$$

$$\therefore\ d(cos\,\theta_0) = \frac{d\left(v^2\right)}{2v_0 V} \ \Rightarrow\ \left|\sin\theta_0 d\theta_0\right| = \frac{d\left(v^2\right)}{2v_0 V}$$

$$\Rightarrow \frac{1}{2}\left|\sin\theta_0 d\theta_0\right| = \frac{d\left(\frac{1}{2}v^2\right)}{2v_0 V}$$

$$\Rightarrow \frac{1}{2}\left|\sin\theta_0 d\theta_0\right| = \frac{d\left(\frac{1}{2}mv^2\right)}{2mv_0V} \tag{4.5}$$

Using the kinetic energy $T = \frac{1}{2}mv^2$, where m is either m_1 or m_2 depending on which particle is under consideration:

$\therefore$ From eq.(4.3) and (4.5) ,required distribution $= \frac{dT}{2mv_0V}$

- In Lab frame ,by eq.(4.4)

  $v_{\min} = |v_0 - V|$ and $v_{\max} = v_0 + V$

The kinetic energy can take values between $T_{min} = \frac{1}{2}m(v_0 - V)^2$ and $T_{max} = \frac{1}{2}m(v_0 + V)^2$. The particles are distributed uniformly over this range.

Example 4.1 Determine the effective cross-section(in CM frame) for scattering of a particle from a perfectly rigid sphere of radius a (i.e. when the interaction is such that $U = \infty$ for $r < a$, and $U = 0$ for $r > a$,

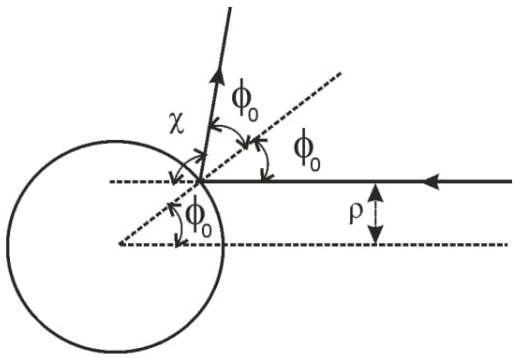


Figure 4.3

Sol. Since a particle moves freely outside the sphere and cannot penetrate into it, the path consists of two straight lines symmetrical about the radius to the point where particle strikes the sphere. It is evident from the figure(4.3):

$$\chi + 2\varphi_0 = \pi \tag{4.6}$$

Where χ is deviation angle (angle between final and initial direction of motion of the particle). We have

$$\rho = a\sin\varphi_0 = a\sin\left(\frac{\pi}{2} - \frac{\chi}{2}\right) = a\cos\frac{\chi}{2} \tag{4.7}$$

Area between two circles of radii ρ and $\rho + d\rho$ is $d(\pi\rho^2)$ i.e. $2\pi\rho d\rho$

Effective cross section $\boxed{d\sigma = 2\pi\rho d\rho}$

$$d\sigma = 2\pi\rho\left|\frac{d\rho}{d\chi}\right| d\chi \tag{4.8}$$

Solid angle between the cones with vertical angles χ and $\chi + d\chi$ is

$$d\Omega = \frac{dA}{r^2} = \frac{2\pi r\sin\chi\,(rd\chi)}{r^2}$$

$$d\Omega = 2\pi\sin\chi\, d\chi \tag{4.9}$$

$$\Rightarrow d\chi = \frac{d\Omega}{2\pi\sin\chi}$$

From eqs.(4.8) and(4.9)

$$\therefore\ d\sigma = \frac{\rho}{\sin\chi}.\left|\frac{d\rho}{d\chi}\right| d\Omega \tag{4.10}$$

Using eq.(4.10)and(4.7)

$$d\sigma = \frac{a\cos\frac{\chi}{2}}{2\sin\frac{\chi}{2}\cos\frac{\chi}{2}} \times \left|-a\times\frac{1}{2}\sin\frac{\chi}{2}\right| d\Omega$$

$$\Rightarrow d\sigma = \frac{1}{4}a^2 d\Omega \tag{4.11}$$

Let the scattering is isotropic in the C-system.

On integrating $d\sigma$ over all angles, we find that the total cross section is $\sigma = \pi a^2$ $\left(\because \boxed{\oint d\Omega = 4\pi}\right)$.

This result is in accordance with the fact that the "impact area" which the particle must strike in order to be scattered is simply the cross-section area of the sphere.

4.3 Elastic Collisions

A collision between two particles is said to be elastic if it involves no changes in their internal state i.e. internal energy of the each colliding particle after the

collision is equal to its initial internal energy.

➢ The collision is most simply described in a frame of reference in which the center of mass of the two particles is at rest (the C-system).

We distinguish by the suffix C the value of quantities in that C system and suffix L the value of quantities in that L system.

➢ **In Centre of mass frame:**

Let $\vec{r}_{1C}$ and $\vec{r}_{2C}$ denote the position vectors of particles in CM frame. Let

$$\vec{r} = \vec{r}_{1C} - \vec{r}_{2C} \tag{4.12}$$

be the relative position vector(position vector of the first particle with respect to second particle). Let the origin be at the centre of mass in CM frame ,

$$\vec{r}_{CM,C} = \frac{m_1 \vec{r}_{1C} + m_2 \vec{r}_{2C}}{m_1 + m_2} = \vec{0} \text{ i.e. } m_1 \vec{r}_{1C} + m_2 \vec{r}_{2C} = \vec{0} \tag{4.13}$$

Solving (4.12) and (4.13) we get, $\boxed{\vec{r}_{1C} = \frac{m_2 \vec{r}}{m_1 + m_2}, \vec{r}_{2C} = -\frac{m_1 \vec{r}}{m_1 + m_2}}$ (4.14)

Differentiating the equation (4.12)

$$\frac{d\vec{r}}{dt} = \frac{d\vec{r}_{1C}}{dt} - \frac{d\vec{r}_{2C}}{dt} \tag{4.15}$$

Let $\vec{u}_{1C} = \frac{d\vec{r}_{1C}}{dt}$ = velocity of the first particle in CM frame before the collision

$\vec{u}_{2C} = \frac{d\vec{r}_{2C}}{dt}$ = velocity of the second particle in CM frame before the collision

$\vec{u}_{rel,C} = \frac{d\vec{r}}{dt} = \vec{u}_{1C} - \vec{u}_{2C}$ = Velocity of the first particle with respect to second particle in CM frame before the collision= initial relative velocity in CM frame

Since relative position $\vec{r} = \vec{r}_{1C} - \vec{r}_{2C}$ is same in both CM and L frames i.e. vector $\vec{r}$ is same in both CM and L frames i.e. $\vec{r} = \vec{r}_{1C} - \vec{r}_{2C} = \vec{r}_{1L} - \vec{r}_{2L}$ (where $\vec{r}_{1L}$ and $\vec{r}_{2L}$ denote the position vectors of particles in L frame)

So $\frac{d\vec{r}}{dt}$ represents relative velocity of particles in CM frame as well as in L frame .

$$\therefore \frac{d\vec{r}}{dt} = \vec{u}_{rel,C} = \vec{u}_{rel,L}$$

Let $\vec{u}_{rel,C} = \vec{u}_{rel,L} = \vec{u}_{rel}$ (4.16)

Then $\vec{u}_{1L} = \frac{d\vec{r}_{1L}}{dt}$ = velocity of the first particle in L frame before the collision

$\vec{u}_{2L} = \frac{d\vec{r}_{2L}}{dt}$ = velocity of the second particle in L frame before the collision

$\because \ \vec{r} = \vec{r}_{1C} - \vec{r}_{2C} = \vec{r}_{1L} - \vec{r}_{2L}$

$$\therefore \vec{u}_{rel,L} = \frac{d\vec{r}}{dt} = \frac{d\vec{r}_{1L}}{dt} - \frac{d\vec{r}_{2L}}{dt} = \vec{u}_{1L} - \vec{u}_{2L} \quad (4.17)$$

By eq.(4,16) $\vec{u}_{rel} = \vec{u}_{1L} - \vec{u}_{2L}$ (4.18)

- ***In C-system total momentum of the system is zero*** .
- After differentiating the eq(4.13)we have

$$m_1 \vec{u}_{1C} + m_2 \vec{u}_{2C} = \vec{0} \quad (4.19)$$

differentiating the eq(4.14)we have

$$\vec{u}_{1C} = \frac{m_2 \vec{u}_{rel}}{m_1 + m_2} = \frac{m_2(\vec{u}_{1L} - \vec{u}_{2L})}{m_1 + m_2}, \quad \vec{u}_{2C} = -\frac{m_1 \vec{u}_{rel}}{m_1 + m_2} = -\frac{m_1(\vec{u}_{1L} - \vec{u}_{2L})}{m_1 + m_2}$$

- ***In C-system total momentum of the system is zero by the law of conservation of momentum, the momenta of the two particles remain equal and opposite after collision***, and are also unchanged in magnitude by the law of conservation of energy. Thus, in the C-system the collision simply rotates the velocities, which remain opposite in direction and unchanged in magnitude. If we denote $\hat{n}_0$ a unit vector in the direction of the velocity of the particle m_1 after collision, then the velocities of the two particles after the collision

$$\vec{v}_{1C} = \frac{m_2 u_{rel}}{m_1 + m_2} \hat{n}_0 \ , \vec{v}_{2C} = -\frac{m_1 u_{rel}}{m_1 + m_2} \hat{n}_0 \quad , \quad (4.20)$$

In order to return to the L-system, we must add to these expressions with the velocity $\vec{V}$ of the CM. where $\vec{V} = \frac{m_1 \vec{u}_{1L} + m_2 \vec{u}_{2L}}{m_1 + m_2}$, = Velocity of CM of the system with respect to L frame. By momentum conservation velocity of CM before and

after the collision remains same. Therefore, the velocities in the L-system after the collision are therefore:

➢ Velocity of the particle in L frame=(velocity of CM)+(Velocity of the particle with respect to CM)

So $\vec{v}_{1L} = \vec{V} + \vec{v}_{1C}$

Using (4.20) we have $\vec{v}_{1L} = \dfrac{m_1\vec{u}_{1L} + m_2\vec{u}_{2L}}{m_1 + m_2} + \dfrac{m_2 u_{rel}}{m_1 + m_2}\hat{n}_0$

$$\Rightarrow \vec{v}_{1L} = \frac{\vec{p}_{1L} + \vec{p}_{2L}}{m_1 + m_2} + \frac{m_2 u_{rel}}{m_1 + m_2}\hat{n}_0 \qquad (4.21)$$

and $\vec{v}_{2L} = \vec{V} + \vec{v}_{2C}$

$$\Rightarrow \vec{v}_{2L} = \frac{m_1\vec{u}_{1L} + m_2\vec{u}_{2L}}{m_1 + m_2} - \frac{m_1 u_{rel}}{m_1 + m_2}\hat{n}_0$$

$$\Rightarrow \vec{v}_{2L} = \frac{\vec{p}_{1L} + \vec{p}_{2L}}{m_1 + m_2} - \frac{m_1 u_{rel}}{m_1 + m_2}\hat{n}_0 \qquad (4.22)$$

Multiply (4.21) by m_1 we get momentum of the first particle after the collision

$$\therefore \vec{p}'_{1L} = mu_{rel}\,\hat{n}_0 + \frac{m_1}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right) \quad \text{Where } m = \frac{m_1 m_2}{m_1 + m_2}$$

and (4.22) by m_2, we get we get momentum of the second particle after the collision $\vec{p}'_{2L} = -mu_{rel}\,\hat{n}_0 + \dfrac{m_2}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right)$ (4.23)

The direction of the vector $\hat{n}_0$ depends on the law of interaction of the particles and on their relative position during the collision.

The result obtained in (4.22) and (4.23) may be interpreted geometrically. We draw a circle of radius mu_{rel} and use the construction as shown in figure(4.4),(4.5). If the unit vector $\hat{n}_0$ is along OC where $\overrightarrow{OC} = mu_{rel}\,\hat{n}_0$,

$$\overrightarrow{AO} = \frac{m_1}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right) \text{ and } \overrightarrow{OB} = \frac{m_2}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right)$$

the vectors AC and CB give the momenta $\vec{p}'_{1L}$ and $\vec{p}'_{2L}$ respectively. When $\vec{p}_{1L}$ and $\vec{p}_{2L}$ are given, the radius of the circle and points A and B are fixed, but the point C may be anywhere on the circle.

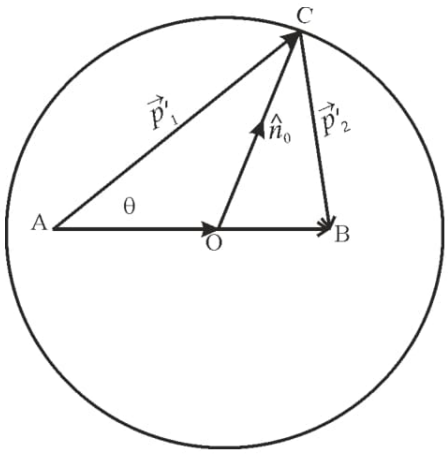


Figure 4.4

Now consider the special case where one of the particles (m_2 , say) is at rest (i.e. $\vec{p}_{2L} = 0$) before the collision.In that case the distance

$$OB = \frac{m_2}{m_1 + m_2}(p_{1L} + 0) = \frac{m_2 m_1 v_{1L}}{m_1 + m_2} = m v_{1L} \tag{4.24}$$

$\because u_{2L} = 0$ By eq. $\overrightarrow{OC} = m u_{rel}\,\hat{n}_0 = m\left|\vec{u}_{1L} - \vec{u}_{2L}\right|\hat{n}_0 \Rightarrow OC = m u_{1L}$ (4.25)

Thus OB equal to the radius(OC), i.e. B lies on the circle{see figure(4.5)and(4.6)}

Here $\overrightarrow{AB} = \overrightarrow{AO} + \overrightarrow{OB} = \frac{m_1}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right) + \frac{m_2}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right)$

$$\because u_{2L} = 0 \qquad \therefore \overrightarrow{AB} = \vec{p}_{1L} + \vec{p}_{2L} = \vec{p}_{1L} \tag{4.26}$$

Thus the vector $\overrightarrow{AB}$ is equal to the momentum $\vec{p}_{1L}$ of particle m_1 before the collision.

$$\because \overrightarrow{AO} = \frac{m_1}{m_1 + m_2}\left(\vec{p}_{1L} + \vec{p}_{2L}\right) \;\&\; u_{2L} = 0$$

$$\therefore AO = \frac{m_1 m_1}{m_1 + m_2} u_{1L} = \frac{m_1 m_2}{m_1 + m_2} u_{1L}\left(\frac{m_1}{m_2}\right) = m u_{1L}\left(\frac{m_1}{m_2}\right) \tag{4.27}$$

By eq.(4.25) $OC = m u_{1L} \;\; \therefore AO = OC\left(\frac{m_1}{m_2}\right)$ (4.28)

The point A lies inside(AO<OC) or outside(AO>OC) the circle, according as $m_1 < m_2$ or $m_1 > m_2$.

By eq.(4.24) $OB = mv_{1L}$ $\because$ $\dfrac{AO}{OB} = \dfrac{m_1}{m_2}$ (4.29)

The corresponding diagrams are shown in the figures given below:

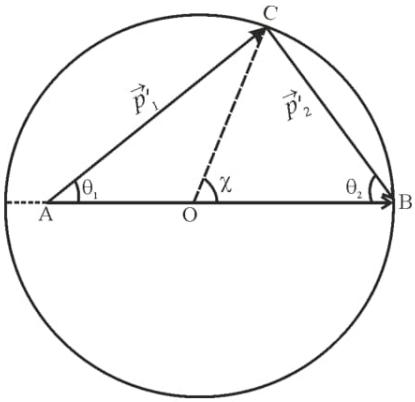


Figure 4.5

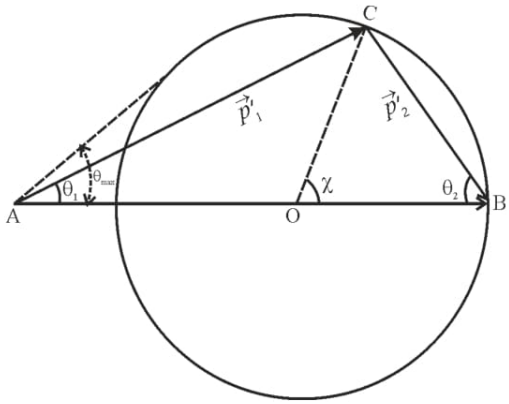


Figure 4.6

By eq.(4.26), $\vec{AB} = \vec{p}_{1L}$,So incident particle moves along AB direction. Vector AC represents the momentum $\vec{p}'_{1L}$ of the first particle after the collision in L frame. Therefore the first particle scattered by an angle θ_1 in Lab frame. In CM Frame, the first particle scattered by an angle χ

$$\tan\theta_1 = \frac{OC\sin\chi}{AO + OC\cos\chi} = \frac{\sin\chi}{\frac{AO}{OC} + \cos\chi} = \frac{\sin\chi}{\frac{m_1}{m_2} + \cos\chi} \quad \left\{ \because By\, eq.(4.29)\, AO = OC\left(\frac{m_1}{m_2}\right) \right.$$

$$\therefore \tan\theta_1 = \frac{m_2\sin\chi}{m_1 + m_2\cos\chi} \qquad (4.30)$$

Here after collision direction of motion of the second particle makes an angle θ_2 with direction of motion of the incident particle. $\theta_2 = \dfrac{1}{2}(\pi - \chi)$ (4.31)

- We may give also the formulae for the magnitudes of the velocities of the two particles after the collision, likewise expressed in terms of χ :

$$AC^2 = AO^2 + OC^2 + 2AO(OC)\cos\chi$$

By eq.(4.29)

$$AC^2 = OC^2\left(\frac{m_1}{m_2}\right)^2 + OC^2 + 2OC\left(\frac{m_1}{m_2}\right)(OC)\cos\chi$$

$$\Rightarrow AC = OC\sqrt{\left(\frac{m_1}{m_2}\right)^2 + 1 + 2\left(\frac{m_1}{m_2}\right)\cos\chi}$$

$$\Rightarrow AC = OC\frac{1}{m_2}\sqrt{m_1^2 + m_2^2 + 2m_1m_2\cos\chi}$$

By eq(4.25)

$$AC = mu_{1L}\frac{1}{m_2}\sqrt{m_1^2 + m_2^2 + 2m_1m_2\cos\chi}$$

$$\Rightarrow AC = \frac{m_1}{m_1 + m_2}u_{1L}\sqrt{m_1^2 + m_2^2 + 2m_1m_2\cos\chi} \quad \because m = \frac{m_1m_2}{m_1 + m_2}$$

$$\Rightarrow m_1v_{1L} = \frac{m_1}{m_1 + m_2}u_{1L}\sqrt{m_1^2 + m_2^2 + 2m_1m_2\cos\chi} \quad \because AC = p'_{1L}$$

$$\Rightarrow v_{1L} = \frac{\sqrt{m_1^2 + m_2^2 + 2m_1m_2\cos\chi}}{m_1 + m_2}u_{1L} \quad , \tag{4.32}$$

From figure (4.5)

$$BC^2 = OB^2 + OC^2 - 2OB(OC)\cos\chi$$

By eq.(4.28)and(4.29),OB=OC

$$\Rightarrow BC^2 = OC^2 + OC^2 - 2OC(OC)\cos\chi$$

$$\Rightarrow BC^2 = OC^2(2)(1-\cos\chi)$$

$$\Rightarrow BC = 2OC\sin\frac{\chi}{2}$$

$$\Rightarrow m_2v_{2L} = 2OC\sin\frac{\chi}{2}$$

By eq.(4.25) , $OC = mu_{1L}$

$$\Rightarrow m_2v_{2L} = \frac{2m_1m_2}{m_1 + m_2}u_{1L}\sin\frac{\chi}{2}$$

$$\therefore v_{2L} = \frac{2m_1}{m_1 + m_2}u_{1L}\sin\frac{\chi}{2} \tag{4.33}$$

From figure(4.5) it is obvious that if point A lies on the circle then $\theta_1 + \theta_2 = \frac{\pi}{2}$

Evidently if A lies inside the circle $(i.e.\ m_1 < m_2)$ then $\angle ACB < \frac{\pi}{2}$ $,\therefore \theta_1 + \theta_2 > \frac{\pi}{2}$

If A lies outside the circle $(i.e.\ m_1 > m_2)$ then $\angle ACB > \frac{\pi}{2}$ $,\therefore \theta_1 + \theta_2 < \frac{\pi}{2}$

If $m_1 > m_2$, the particle m_1 can be deflected only through an angle not exceeding θ_{max} from its original direction(AC becomes tangent to circle), then by right angle triangle $\sin\theta_{\max} = \frac{OC}{OA} = \frac{m_2}{m_1}$ $\{By$ eq.(4.28)$AO = OC\left(\frac{m_1}{m_2}\right)$

- The collision of two particles of equal mass, of which one is initially at rest, is especially simple: in that case byeq.(4.28),(4.29)AO=OC=OB i.e. both A and C lie on the circle.

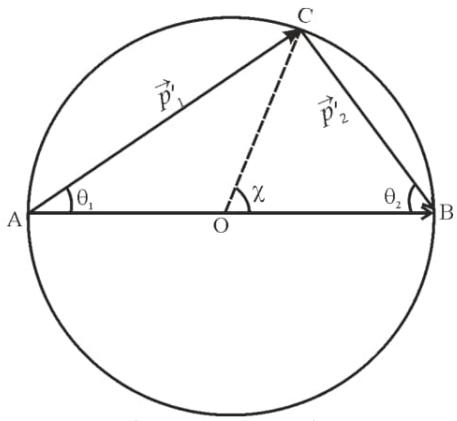


Figure 4.7

$\because \angle OAC = \angle ACO,\ \ \therefore \angle OAC + \angle ACO = \chi, \therefore \theta_1 = \frac{\chi}{2}, \theta_2 = \frac{1}{2}(\pi - \chi)$

By eq.(4.32),(4.33) $v_{1L} = u_{1L}\cos\frac{\chi}{2}$ *and* $v_{2L} = u_{1L}\sin\frac{\chi}{2}$

From figure(4.7) it is obvious that if the point A lies on the circle then $\theta_1 + \theta_2 = \frac{\pi}{2}$ i.e. after the collision the particles move at right angles to each other.

4.4 Rutherford's Formula

One of the most imported applications of the formulae derived above is to the scattering of charged particles in a coulomb field. A particle is scattered by an angle χ and impact parameter is ρ and$U = \frac{\alpha}{r}$

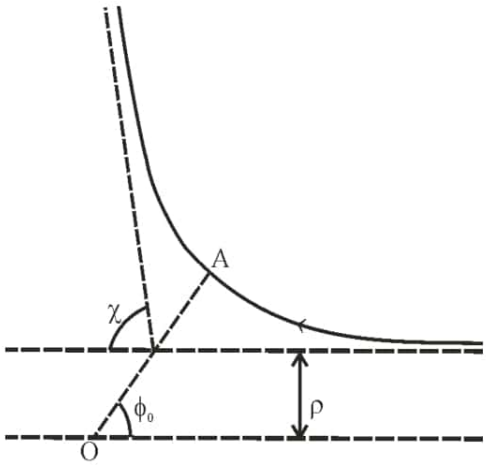


Figure 4.8

From previous chapter, using eq.(3.10) angle $\phi_0 = \int_{r_{min}}^{\infty} \frac{\frac{M}{r^2}dr}{\sqrt{\{2m[E-U(r)]\}-\frac{M^2}{r^2}}}$

$E = \frac{1}{2}mv_\infty^2$, angular momentum $M = m\rho v_\infty$

$$\phi_0 = \int_{r_{\min}}^{\infty} \frac{\frac{m\rho v_\infty}{r^2}dr}{\sqrt{\left\{2m\left[\frac{1}{2}mv_\infty^2 - U\right]\right\}-\frac{(m\rho v_\infty)^2}{r^2}}}$$

$$\phi_0 = \int_{r_{\min}}^{\infty} \frac{\frac{\rho}{r^2}dr}{\sqrt{\left[1-\frac{\rho^2}{r^2}-\frac{2U}{mv_\infty^2}\right]}} = \int_{r_{\min}}^{\infty} \frac{\frac{\rho}{r^2}dr}{\sqrt{\left[1-\frac{\rho^2}{r^2}-\frac{2}{mv_\infty^2}\frac{\alpha}{r}\right]}}$$

$$= -\int_{r_{\min}}^{\infty} \frac{\rho dx}{\sqrt{\left[1-\rho^2x^2-\frac{2}{mv_\infty^2}\alpha x\right]}} \quad \left\{Let\ \frac{1}{r} = x \Rightarrow -\frac{dr}{r^2} = dx\right\}$$

$$= -\int_{r_{\min}}^{\infty} \frac{dx}{\sqrt{\left[\frac{1}{\rho^2}-x^2-\frac{2}{mv_\infty^2\rho^2}\alpha x\right]}}$$

$$= -\int_{r_{\min}}^{\infty} \frac{dx}{\sqrt{\left[\frac{1}{\rho^2} - \left(x + \frac{\alpha}{mv_\infty^2\rho^2}\right)^2 + \left(\frac{\alpha}{mv_\infty^2\rho^2}\right)^2\right]}}$$

$$= -\int_{r_{\min}}^{\infty} \frac{dx}{\sqrt{\left[\left\{\frac{1}{\rho}\sqrt{1+\left(\frac{\alpha}{mv_\infty^2\rho}\right)^2}\right\}^2 - \left(x + \frac{\alpha}{mv_\infty^2\rho^2}\right)^2\right]}}$$

$$\phi_0 = \cos^{-1}\left\{\frac{x + \frac{\alpha}{mv_\infty^2\rho^2}}{\frac{1}{\rho}\sqrt{1+\left(\frac{\alpha}{mv_\infty^2\rho}\right)^2}}\right\}_{x_1}^{x_2}$$

$$\Rightarrow \phi_0 = \cos^{-1}\left\{\frac{\frac{1}{r} + \frac{\alpha}{mv_\infty^2\rho^2}}{\frac{1}{\rho}\sqrt{1+\left(\frac{\alpha}{mv_\infty^2\rho}\right)^2}}\right\}_{r_{\min}}^{\infty}$$

$$\Rightarrow \varphi_0 = \cos^{-1}\left\{\frac{\frac{\alpha}{mv_\infty^2\rho^2}}{\frac{1}{\rho}\sqrt{1+\left(\frac{\alpha}{mv_\infty^2\rho}\right)^2}}\right\} - \cos^{-1}\left\{\frac{\frac{1}{r_{\min}} - \frac{\alpha}{mv_\infty^2\rho^2}}{\frac{1}{\rho}\sqrt{1+\left(\frac{\alpha}{mv_\infty^2\rho}\right)^2}}\right\} \qquad (4.34)$$

By angular momentum conservation $\boxed{mv_\infty\rho = mv_{\max}r_{\min}} \Rightarrow v_{\max} = \frac{v_\infty\rho}{r_{\min}}$ (4.35)

By energy conservation $\frac{1}{2}mv_\infty^2 + \frac{\alpha}{\infty} = \frac{1}{2}mv_{\max}^2 + \frac{\alpha}{r_{\min}}$

$$\Rightarrow \frac{1}{2}mv_\infty^2 = \frac{1}{2}m\left(\frac{v_\infty\rho}{r_{\min}}\right)^2 + \frac{\alpha}{r_{\min}} \qquad \left\{\because v_{\max} = \frac{v_\infty\rho}{r_{\min}}\right.$$

$$\Rightarrow \frac{1}{2}m\frac{v_\infty^2\rho^2}{r_{\min}^2} + \frac{\alpha}{r_{\min}} - \frac{1}{2}mv_\infty^2 = 0$$

$$\Rightarrow \frac{1}{r_{\min}} = \frac{-\alpha + \sqrt{\alpha^2 + m^2 v_\infty^4 \rho^2}}{m v_\infty^2 \rho^2} = -\frac{\alpha}{m v_\infty^2 \rho^2} + \frac{1}{\rho}\sqrt{1 + \left(\frac{\alpha}{m v_\infty^2 \rho}\right)^2}$$

Putting this value of $\frac{1}{r_{\min}}$ in eq.(4.34)

$$\phi_0 = \cos^{-1}\left\{\frac{\frac{\alpha}{m v_\infty^2 \rho^2}}{\frac{1}{\rho}\sqrt{1 + \left(\frac{\alpha}{m v_\infty^2 \rho}\right)^2}}\right\} - \cos^{-1}(1)$$

$$\Rightarrow \phi_0 = \cos^{-1}\left\{\frac{\frac{\alpha}{m v_\infty^2 \rho^2}}{\frac{1}{\rho}\sqrt{1 + \left(\frac{\alpha}{m v_\infty^2 \rho}\right)^2}}\right\} \Rightarrow \cos\phi_0 = \frac{\left(\frac{\alpha}{m v_\infty^2 \rho}\right)}{\sqrt{1 + \left(\frac{\alpha}{m v_\infty^2 \rho}\right)^2}}$$

Therefore $\tan\phi_0 = \frac{1}{\left(\frac{\alpha}{m v_\infty^2 \rho}\right)} \Rightarrow \rho^2 = \frac{\alpha^2}{m^2 v_\infty^4}\tan^2\varphi_0$

From figure(4.8) $\phi_0 + \phi_0 + \chi = \pi \Rightarrow \phi_0 = \frac{1}{2}(\pi - \chi)$

Where χ is the scattering angle

Now, using $\varphi_0 = \frac{1}{2}(\pi - \chi)$ (4.36)

$$\Rightarrow \rho^2 = \frac{\alpha^2}{m^2 v_\infty^4}\cot^2\frac{\chi}{2} \Rightarrow \rho = \frac{\alpha}{m v_\infty^2}\cot\frac{\chi}{2} \tag{4.37}$$

$$\Rightarrow \left|\frac{d\rho}{d\chi}\right| = \frac{\alpha}{2 m v_\infty^2}\left|\cos ec^2\frac{\chi}{2}\right| \tag{4.38}$$

From eq.(4.8)effective cross section $d\sigma = 2\pi\rho\left|\frac{d\rho}{d\chi}\right|d\chi$

$$d\sigma = \pi\left(\frac{\alpha}{m v_\infty^2}\right)^2 \frac{\cos\frac{\chi}{2}\, d\chi}{\sin^3\frac{\chi}{2}} \tag{4.39}$$

From eq.(4.10), $d\sigma = \frac{\rho}{\sin\chi}.\left|\frac{d\rho}{d\chi}\right| d\Omega$.

Using eq.(4.37)and(4.38)

$$d\sigma = \frac{\frac{\alpha}{mv_\infty^2}\cot\frac{\chi}{2}}{\sin\chi}.\frac{\alpha}{2mv_\infty^2}\cos ec^2\frac{\chi}{2}d\Omega \quad .$$

Using $\sin\chi = 2\sin\frac{\chi}{2}\cos\frac{\chi}{2}$

or $$\boxed{d\sigma = \left(\frac{\alpha}{2mv_\infty^2}\right)^2 \frac{d\Omega}{\sin^4\frac{\chi}{2}}} \qquad (4.40)$$

This is Rutherford's formula. It may be noted that the effective cross section is independent of the sign of α, so that the result is equally valid for repulsive and attractive coulomb fields.

- Formula (4.40) gives the effective cross-section in the frame of reference in which the centre of mass of the colliding particles is at rest.
- The transformation to the laboratory system is effected by means formulae(4.30) and (4.31)

$$\tan\theta_1 = \frac{m_2\sin\chi}{m_1 + m_2\cos\chi},$$

$$\theta_2 = \frac{1}{2}(\pi - \chi) \qquad \therefore \ \chi = \pi - 2\theta_2 \qquad \therefore$$

$$\cos\frac{\chi}{2} = \cos\left(\frac{\pi}{2} - \theta_2\right) = \sin\theta_2 \qquad (4.41)$$

From eq.(4.39), $d\sigma = \pi\left(\frac{\alpha}{mv_\infty^2}\right)^2 \frac{\cos\frac{\chi}{2}d\chi}{\sin^3\frac{\chi}{2}}$

$$\therefore \ d\sigma_2 = \pi.\left(\frac{\alpha}{mv_\infty^2}\right)^2\left|\frac{\sin\theta_2}{\cos^3\theta_2}(-2d\theta_2)\right|$$

$$= .\left(\frac{\alpha}{mv_\infty^2}\right)^2 \frac{(2\pi\sin\theta_2 d\theta_2)}{\cos^3\theta_2} = \left(\frac{\alpha}{mv_\infty^2}\right)^2 \frac{d\Omega_2}{\cos^3\theta_2} \qquad (4.42)$$

The same transformation for the incident particles leads, in general, to a very complex formula. We shall find it for the following two particular cases:

Case-I. If the mass m_2 of the scattering particle is large compared with the mass m_1 of the scattered particle, then from eq.(4.30) and (4.31)

$$\left(\because \tan\theta_1 = \frac{m_2 \sin\chi}{m_1 + m_2\cos\chi} \approx \frac{m_2\sin\chi}{m_2\cos\chi} = \tan\chi \right)$$

$$\chi \approx \theta_1, m = \frac{m_1 m_2}{m_1 + m_2} \approx m_1$$

By eq.(4.40), $d\sigma = \left(\frac{\alpha}{2mv_\infty^2}\right)^2 \frac{d\Omega}{\sin^4\frac{\chi}{2}}$

$\therefore\ d\sigma_1 = \left(\frac{\alpha}{4E_1}\right)^2 \frac{d\Omega_1}{\sin^4\frac{\theta_1}{2}}$, where $E_1 = \frac{1}{2}m_1 v_\infty^2$ is the energy of the incident particle.

Case-II. If $m_1 = m_2$, $m = \frac{1}{2}m_1$, then $\chi = 2\theta$,

$$\left(by(4.30),(4.31) \because \tan\theta_1 = \frac{\sin\chi}{1+\cos\chi} = \frac{2\sin\frac{\chi}{2}\cos\frac{\chi}{2}}{2\cos^2\frac{\chi}{2}} \Rightarrow \theta_1 = \frac{\chi}{2} \right)$$

By eq.(4.39) $d\sigma = \pi\left(\frac{\alpha}{mv_\infty^2}\right)^2 \frac{\cos\frac{\chi}{2}d\chi}{\sin^3\frac{\chi}{2}}$

$$\therefore\ d\sigma_1 = \pi.\left(\frac{\alpha}{\frac{1}{2}m_1 v_\infty^2}\right)^2 \frac{\cos\theta_1 . 2d\theta_1}{\sin^3(\theta_1)}$$

$$= 2\pi.\left(\frac{\alpha}{E_1}\right)^2 . \frac{\cos\theta_1\, d\theta_1}{\sin^3\theta_1}$$

$$= \left(\frac{\alpha}{E_1}\right)^2 .\cos\theta_1 \frac{d\Omega_1}{\sin^4\theta_1} \qquad \{\because d\Omega = 2\pi\sin\theta d\theta \qquad (4.43)$$

If the particles are entirely identical, that which was initially at rest cannot be distinguished after collision. The total effective cross section for all particles is

obtained by adding $d\sigma_1$ and $d\sigma_2$ and replacing θ_1 and θ_2 by their common value θ,From eq.(4.42),(4.43)

$$d\sigma = \left(\frac{\alpha}{E_1}\right)^2 \left(\frac{1}{\sin^4\theta} + \frac{1}{\cos^4\theta}\right)\cos\theta\, d\Omega$$

Using (4.39) $d\sigma = \pi\left(\frac{\alpha}{mv_\infty^2}\right)^2 \cos\frac{\chi}{2}\frac{d\chi}{\sin^3\frac{\chi}{2}}$, we can determine the distribution of the scattered particles with respect to the energy lost in the collision.

- When m_1 and m_2 are arbitrary $\begin{pmatrix} m_1 : \text{scattered particle} \\ m_2 : \text{scattering particle} \end{pmatrix}$ the velocity acquired by m_2 is given in terms of the angle of scattering (in the C-system)by eq.(4.33)

$$v_{2L} = \frac{2m_1}{m_1 + m_2} u_{1L} \sin\frac{\chi}{2}$$

$$v_{2L} = \frac{2m_1}{m_1 + m_2} u_\infty . \sin\frac{\chi}{2}$$

- The energy acquired by m_2 and lost by m_1 is therefore

$$\in = \frac{1}{2} m_2 v_{2L}^2 = \frac{1}{2} m_2 . \frac{4m_1^2}{(m_1 + m_2)^2} u_\infty^2 . \sin^2\frac{\chi}{2} = \frac{2}{m_2} m^2 u_\infty^2 . \sin^2\frac{\chi}{2} \qquad \because m = \frac{m_1 m_2}{m_1 + m_2}$$

$$\Rightarrow \in = \left(\frac{2m^2}{m_2}\right) u_\infty^2 . \sin^2\frac{\chi}{2} \qquad \Rightarrow \sin\frac{\chi}{2} = \left(\frac{m_2}{2m^2}\right)^{\frac{1}{2}} \frac{1}{u_\infty} \in^{\frac{1}{2}}$$

$$\Rightarrow \frac{1}{2}\cos\frac{\chi}{2} . d\chi = \left(\frac{m_2}{2m^2}\right)^{\frac{1}{2}} \frac{1}{u_\infty} . \frac{1}{2} \in^{-\frac{1}{2}} d \in$$

Substituting above values $\cos\frac{\chi}{2} . d\chi$ and $\sin\frac{\chi}{2}$ in $d\sigma = \pi\left(\frac{\alpha}{mv_\infty^2}\right)^2 \cos\frac{\chi}{2}\frac{d\chi}{\sin^3\frac{\chi}{2}}$

$$d\sigma = \pi . \left(\frac{\alpha}{mv_\infty^2}\right)^2 . \left(\frac{m_2}{2m^2}\right)^{\frac{1}{2}} . \frac{1}{v_\infty} . \in^{-\frac{1}{2}} d \in . \left(\frac{2m^2}{m_2}\right)^{3/2} v_\infty^3 \in^{-3/2}$$

$$= \pi . \left(\frac{\alpha}{mv_\infty^2}\right)^2 . \left(\frac{2m^2}{m_2}\right) v_\infty^2 . \frac{1}{\in^2} d \in$$

$$d\sigma = 2\pi . \left(\frac{\alpha^2}{m_2 v_\infty^2}\right) \frac{d \in}{\in^2}$$

This is the required formula . It gives the effective cross-section as a function of the energy lose $\in$, which takes values from zero to $\in_{max} = \frac{2m^2}{m_2} v_\infty^2$

($\because \in = \left(\frac{2m^2}{m_2}\right) u_\infty^2 . \sin^2 \frac{\chi}{2}$ & $\chi = 180^\circ$, back scattering)

Example 4.2 Determine the effective cross-section as a function of the energy $\in$ lost by a scattered particle from a perfectly rigid sphere of radius a (i.e. $\cup = \infty$ for $r < a$, and $\cup = 0$ for $r > a$).

Sol. The energy lost by a particle of mass m_1 is equal to that gained by the sphere of mass m_2.

$$\in = \mathrm{E}_2' = \frac{1}{2} m_2 v_{2L}^2$$

By using eq.(4.33) $v_{2L} = \frac{2m_1}{m_1 + m_2} u_{1L} \sin \frac{\chi}{2}$

$$v_{2L} = \frac{2m_1}{m_1 + m_2} u_\infty \sin \frac{\chi}{2}$$

$$\therefore \quad \in = \frac{1}{2} m_2 \frac{4m_1^2 u_\infty^2}{(m_1 + m_2)^2} \sin^2 \frac{\chi}{2}$$

$$= \frac{2m_1^2 m_2}{(m_1 + m_2)^2} u_\infty^2 . \sin^2 \frac{\chi}{2} = \in_{\max} \sin^2 \frac{\chi}{2}$$

$$\therefore \quad d \in = \in_{\max} .2 \sin \frac{\chi}{2} \cos \frac{\chi}{2} . \frac{1}{2} d\chi = \frac{1}{2} \in_{\max} \sin \chi \, d\chi$$

$$\frac{2d \in}{\in_{\max}} = \sin \chi \, d\chi \qquad (4.44)$$

By eq.(4.9) and (4.11) $d\Omega = 2\pi \sin \chi \, d\chi$, $d\sigma = \frac{1}{4} a^2 d\Omega$

$$\therefore \quad d\sigma = \frac{1}{2} \pi a^2 \sin \chi \, d\chi$$

From eq.(4.44) $\quad d\sigma = \frac{1}{2} \pi a^2 . \frac{2d \in}{\in_{\max}} = \pi a^2 \frac{d \in}{\in_{\max}}$

The scattered particles are uniformly distributed with respect to $\in$ in the range from zero to $\in_{max}$.

4.5 Self Learning Exercise-I

Q.1 In the elastic collision of two particles of equal mass in which one particle at rest is struck by other, the angle of deflection of the two particles is

(A) less than $\frac{\pi}{2}$ (B) more than $\frac{\pi}{2}$

(C) equal to $\frac{\pi}{2}$ (D) more than π

Q.2 In the above problem if $m_1 > m_2$, m_2 is at rest then angle of diversion

(A) $\theta_1 + \theta_2 < \frac{\pi}{2}$ (B) $\theta_1 + \theta_2 > \frac{\pi}{2}$

(C) $\theta_1 + \theta_2 = \pi$ (D) $\theta_1 + \theta_2 > \pi$

Q.3 Establish a relation between scattering angles in laboratory and centre of mass coordinates in a two body scattering problem.

Q.4 What changes ,if any ,would there be in Rutherford scattering if the coulomb force were attractive, instead of repulsive.

Q.5 Determine the effective cross-section for a particle to "fall" to the centre of a field $U = -\frac{\alpha}{r^2}$.

Example 4.3 Determine the effective cross-section for particles of mass m_1 to strike a sphere of mass m_2 and radius R to which they are attracted in accordance with Newton's law.

Sol. The condition for a particle to reach(collide) the sphere is that $r_{min} < R$, where r_{min} is the point on the path which is nearest to the centre of the sphere.

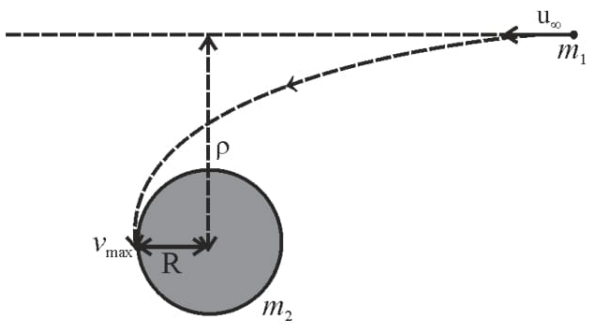


Figure 4.9

We have (reduced mass) $m = \dfrac{m_1 m_2}{m_1 + m_2} \approx m_1$,on the assumption that $m_2 >> m_1$

The greatest possible value of impact parameter ρ is given by $r_{min} = R$;

By angular momentum conservation

$$m_1 u_\infty \rho_{\max} = m_1 v_{\max} r_{\min} \Rightarrow v_{\max} = \frac{u_\infty \rho_{\max}}{r_{\min}} = \frac{u_\infty \rho_{\max}}{R} \tag{4.45}$$

By energy conservation $$\frac{1}{2} m u_\infty^2 - \frac{\alpha}{\infty} = \frac{1}{2} m v_{\max}^2 - \frac{\alpha}{r_{\min}} \tag{4.46}$$

Here $U = -\dfrac{\alpha}{r} = -\dfrac{G m_1 m_2}{r}$

By eq.(4.45) and (4.46)

$$\frac{1}{2} m_1 u_\infty^2 = \frac{1}{2}\, m_1 \frac{v_\infty^2 \rho_{\max}^2}{R^2} - \frac{\alpha}{R}.$$

Where $\alpha = G m_1 m_2$ (G being universal gravitational constant) and. Solving for ρ_{max}^2:

$$\frac{1}{2} \frac{m_1 u_\infty^2 \rho_{\max}^2}{R^2} = \frac{1}{2} m_1 u_\infty^2 + \frac{\alpha}{R}$$

$$\therefore \rho_{\max}^2 = \frac{R^2}{\frac{1}{2} m_1 u_\infty^2} \left(\frac{1}{2} m_1 u_\infty^2 + \frac{\alpha}{R} \right)$$

$$= R^2 + \frac{\alpha}{R} . \frac{R^2}{\frac{1}{2} m_1 u_\infty^2}$$

$$= R^2 \left[1 + \frac{2\alpha}{R\left(m_1 u_\infty^2 \right)} \right]$$

$$\rho_{\max} = R^2 \left[1 + \frac{2 G m_1 m_2}{R\left(m_1 u_\infty^2 \right)} \right] = R^2 \left[1 + \frac{2 G m_2}{R u_\infty^2} \right]$$

$$Cross\text{sec}tion\ \sigma = \int_0^{\rho_{\max}} 2\pi \rho\, d\rho = \pi \rho_{max}^2 = \pi R^2 \left(1 + \frac{2G\, m_2}{R\, u_\infty^2} \right).$$

Where $v_\infty \to \infty \ \ \sigma \Rightarrow \pi R^2$ (geometrical cross section of the sphere.)

Example 4.4 Find the effective cross-section for scattering in a field

$$U=\frac{\alpha}{r^2} \quad where(\alpha>0).$$

Sol. From eq.(3.11) $\varphi_0=\int_{r_{\min}}^{\infty}\frac{Mdr}{r^2\sqrt{2m\left(E-U_{eff}\right)}}$ (4.47)

From eq.(4.6) $2\phi_0+\chi=\pi \Rightarrow \phi_0=\frac{\pi}{2}-\frac{\chi}{2}$

Energy of the particle $E=\frac{1}{2}mu_\infty^2+\frac{\alpha}{\infty^2}=\frac{1}{2}mu_\infty^2$

Angular momentum $M=mv_\infty\rho$ (4.48)

From eq.(3.11) $U_{eff}=U(r)+\frac{M^2}{2mr^2}$

$$U_{eff}=\frac{\alpha}{r^2}+\frac{M^2}{2mr^2} \tag{4.49}$$

Using(4.47),(4.48)and(4.49)

$$\phi_0=\int_{r_{\min}}^{\infty}\frac{mu_\infty\rho\,dr}{r^2\sqrt{2m\left[\frac{1}{2}mu_\infty^2-\frac{\alpha}{r^2}-\frac{m^2u_\infty^2\rho^2}{2mr^2}\right]}}$$

$$=\int_{r_{\min}}^{\infty}\frac{mu_\infty\rho\,dr}{r^2\left[2m\frac{1}{2}mu_\infty^2\left(1-\frac{2\alpha}{mu_\infty^2r^2}-\frac{\rho^2}{r^2}\right)\right]^{\frac{1}{2}}}$$

$$=\int_{r_{\min}}^{\infty}\frac{\rho\,dr}{r^2\left[1-\left(\frac{2\alpha}{mu_\infty^2}+\rho^2\right)\frac{1}{r^2}\right]^{\frac{1}{2}}}$$

Let $\frac{1}{r}=t$ or $-\frac{1}{r^2}dr=dt$

$$\therefore \quad \phi_0=\int-\frac{\rho\,dt}{\sqrt{1-A^2t^2}}, \quad \text{where } A^2=\frac{2\alpha}{mu_\infty^2}+\rho^2 \tag{4.50}$$

$$\phi_0=\frac{\rho}{A}\left[\cos^{-1}(At)\right]_1^2=\frac{\rho}{A}\left[\cos^{-1}\left(\frac{A}{r}\right)\right]_{r_{\min}}^{\infty}$$

$$\varphi_0 = \frac{\rho}{A}\left[\cos^{-1}(0) - \cos^{-1}\left(\frac{A}{r_{\min}}\right)\right] = \frac{\rho}{A}\left[\frac{\pi}{2} - \cos^{-1}\left(\frac{A}{r_{\min}}\right)\right] \qquad (4.51)$$

By angular momentum conservation $mu_\infty \rho = mv_{\max} r_{\min} \Rightarrow v_{\max} = \frac{u_\infty \rho}{r_{\min}}$

By energy conservation $\frac{1}{2}mu_\infty^2 + \frac{\alpha}{\infty^2} = \frac{1}{2}mv_{\max}^2 + \frac{\alpha}{r_{\min}^2}$

$$\frac{1}{2}mu_\infty^2 = \frac{1}{2}m\left(\frac{u_\infty \rho}{r_{\min}}\right)^2 + \frac{\alpha}{r_{\min}^2} \qquad \left\{\because v_{\max} = \frac{u_\infty \rho}{r_{\min}}\right.$$

$$\frac{1}{2}mu_\infty^2 = \frac{1}{2}m\frac{u_\infty^2 \rho^2}{r_{\min}^2} + \frac{\alpha}{r_{\min}^2} \Rightarrow r_{\min}^2 = \frac{2\alpha + mu_\infty^2 \rho^2}{mu_\infty^2}$$

Uing eq.(4.50) $r_{\min} = \sqrt{\frac{2\alpha}{mu_\infty^2} + \rho^2} = A$

From eq.(4.51) $\phi_0 = \frac{\rho}{A}\left[\frac{\pi}{2} - \cos^{-1}\left(\frac{A}{A}\right)\right]$

$$\phi_0 = \frac{\rho}{A}\frac{\pi}{2} \quad ....(4.51)$$

From eq.(4.6) $2\phi_0 + \chi = \pi$

$$\Rightarrow \chi = \pi - 2\phi_0 = \pi - \frac{\rho\pi}{A} = \pi\left(1 - \frac{\rho}{A}\right)$$

$$\Rightarrow \rho = (\pi - \chi)\frac{A}{\pi} \quad , \quad \frac{d\rho}{d\chi} = -\frac{A}{\pi} \qquad (4.52)$$

From eq.(4.10)the effective cross section $d\sigma = \frac{\rho}{\sin\chi}.\left|\frac{d\rho}{d\chi}\right| d\Omega$

Using (4.52) $d\sigma = \frac{(\pi - \chi)\frac{A}{\pi}}{\sin\chi}.\frac{A}{\pi}d\Omega = \frac{A^2}{\pi^2}\frac{(\pi - \chi)}{\sin\chi}d\Omega \qquad (4.53)$

From eq.(4.50),(4.52) $A^2 = \frac{2\alpha}{mu_\infty^2} + \rho^2$

$$A^2 = \frac{2\alpha}{mu_\infty^2} + \left((\pi - \chi)\frac{A}{\pi}\right)^2 \Rightarrow A^2\pi^2 = \frac{2\alpha\pi^2}{mu_\infty^2} + \left[\pi^2 - 2\pi\chi + \chi^2\right]A^2$$

$$0=\frac{2\alpha\pi^2}{mu_\infty^2}+[-2\pi+\chi]\chi A^2 \Rightarrow A^2=\frac{2\alpha\pi^2}{mu_\infty^2}\frac{1}{(2\pi-\chi)\chi}$$

Putting this value in eq.(4.53) we have

$$d\sigma=\frac{2\pi^2\alpha}{mu_\infty^2}\cdot\frac{\pi-\chi}{\chi^2(2\pi-\chi)^2}\cdot\frac{d\Omega}{\sin\chi}$$

4.6 Summary

In this chapter we have studied disintegration of particles in C.M. frame and then transformed these formulae to L-frame. We have scattering cross section for Rutherford scattering. There are several solved problems involving hard sphere scattering etc.

4.7 Glossary

***Elastic collision*:** initial(before collision) and final kinetic energy(after collision) of the system remains same

Spontaneous: happening or done in a natural, often sudden way, or without being forced

4.8 Answers to Self Learning Exercise

Ans.1: C **Ans.2:** A

Ans.5: The particles which "fall" to the centre are those for which $2\alpha < m\rho^2 v_\infty^2$ i.e. for which ρ_{max} does not exceed $\sqrt{\frac{2\alpha}{mv_\infty^2}}$

The effective cross section is

$$\sigma=\int_0^{\rho_{\max}}2\pi\rho\,d\rho=\frac{2\pi\rho_{\max}^2}{2}=\pi\rho_{\max}^2=\frac{2\pi\alpha}{mv_\infty^2}$$

4.9 Exercise

Very Short Answer Type Questions

Q.1 The effective cross-section for scattering of particles from a perfectly rigid sphere of radius a is

(A) a^2 (B) $4\pi a^2$ (C) $\frac{1}{2}a^2$ (D) $\frac{1}{4}a^2$

Q.2 In Rutherford scattering, scattering cross section is proportional to

(A) $\frac{1}{\sin^4\frac{\theta}{2}}$ (B) $\frac{1}{\sin^3\frac{\theta}{2}}$ (C) $\frac{1}{\sin^2\frac{\theta}{2}}$ (D) $\frac{1}{\sin\frac{\theta}{2}}$

Q.3 Define scattering cross section

Short Answer Type Questions

Q.4 What do you mean by the laboratory system and centre of mass system in a two body scattering problem ?

Long Answer Type Questions

Q.5 Find the effective cross-section as a function of the velocity v_∞ for particles scattered in a field $U \sim r^{-n}$.

4.10 Answers to Exercise

Ans.1: D **Ans.2:** A

Ans.5 : As the potential energy is a homogeneous function of order $k = -n$, then similar paths are such that $\rho \sim v^{-2/n}$

or $\rho = v_\infty^{-2/n} f(x)$, the angles of deflection being equal for similar paths.

and $d\sigma = \frac{\rho}{\sin\chi}.\left|\frac{d\rho}{d\chi}\right| d\Omega = v_\infty^{-2/n}\left(v_\infty^{-2/n}\right)\left|\frac{df}{dx}\right| . \frac{d\Omega}{\sin x} \sim v_\infty^{-4/n} d\Omega$

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UNIT- 5
Small Oscillations

Structure of the Unit

5.0 Objectives

5.1 Introduction

5.2 Small oscillations

5.3 Forced Oscillations

5.4 Oscillations of Systems With more than One Degree of Freedom

5.5 Self learning Exercise-I

5.6 Vibrations of Molecules

5.7 Self Learning Exercise-II

5.8 Summary

5.9 Glossary

5.10 Answers to Self Learning Exercises

5.11 Exercise

5.12 Answers to Exercise

References and Suggested Readings

5.0 Objectives

In this chapter we shall focus upon a theory of small oscillations based on Lagrangian formulation .

5.1 Introduction

The theory of small oscillations about the equilibrium position is of importance in molecular spectra, acoustics, vibration of atoms in solids, vibrations of coupled mechanical systems and coupled electrical circuits. If the displacement from the stable equilibrium conditions are small, the motion can be described as that of a system of coupled linear harmonic oscillators with each generalized

coordinate expressed as a function of the different frequencies of vibrations of the system. The problem can be simplified further by transformation of the generalized coordinates to another set of coordinates, each of which undergoes period motion with a well defined single frequency.

5.2 Small oscillations

We consider small oscillations of a mechanical system about a position of stable equilibrium. For simplicity we consider small oscillations of a system with only one degree of freedom. Stable equilibrium corresponds to a position q of the system in which its potential energy $U(q)$ is a minimum.

A movement away from this position results in the setting up of a restoring force $-\frac{dU}{dq}$ which tends to return the system to equilibrium.

Let $q = q_0$ be the equilibrium value of the generalized coordinate.

For small deviations from the equilibrium position, it is sufficient to retain the first non-vanishing term in the expansion of the difference in potential energy $U(q) - U(q_0)$ in powers of $(q - q_0)$. We can write

$\because U(q) = U[q_0 + (q - q_0)]$

By Taylor's series expansion

$$U(q) = U(q_0) + (q - q_0)\left(\frac{dU}{dq}\right)_{q=q_0} + \frac{(q-q_0)^2}{2!}\left(\frac{d^2U}{dq^2}\right)_{q=q_0} + \ldots\ldots$$

At equilibrium position force is zero, so at the position q_0

Force $F = -\left(\frac{dU}{dq}\right)_{q=q_0} = 0$

If we assume $U(q_0) = 0$ then above expression of $U(q)$ becomes

$$U(q) = 0 + (q - q_0).0 + \frac{(q-q_0)^2}{2!}\left(\frac{d^2U}{dq^2}\right)_{q=q_0} + \ldots\ldots$$

After neglecting the higher order terms for small oscillations

$$U(q) = \frac{(q-q_0)^2}{2!}\left(\frac{d^2U}{dq^2}\right)_{q=q_0}$$

If we use the symbol $x = (q - q_0)$, for the deviation of the coordinates from its equilibrium value, we find

$$U(x)=\frac{1}{2}kx^2, where\, k=\left(\frac{d^2U}{dq^2}\right)_{q=q_0}$$

The kinetic energy of a system with one degree of freedom is in general of the form $\frac{1}{2}a(q)\dot{q}^2=\frac{1}{2}a(q)\dot{x}^2$

Here $\dot{x}=\dot{q}-\dot{q}_0=\dot{q}-0=\dot{q}$

We replace the function $a(q)$ by its value at $q=q_0$, in the approximation of small deviation from equilibrium.

Putting $a\,(q_0)=m$, we find $KE=T=\frac{1}{2}m\dot{x}^2$

Lagrangian $L=\frac{1}{2}m\,\dot{x}^2-\frac{1}{2}kx^2$

Here $\frac{\partial L}{\partial \dot{x}}=m\dot{x}$, $\frac{\partial L}{\partial x}=-kx$

The corresponding Lagrange's equations of motion is $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)-\frac{\partial L}{\partial x}=0$

$$\frac{d}{dt}(m\dot{x})-(-kx)=0 \qquad m\,\ddot{x}+kx=0$$

Or $\boxed{\ddot{x}+\omega^2x=0\ , where\ \omega=\sqrt{\frac{k}{m}}}$

Two independent solution of the linear differential equation are $cos\ \omega t$ and $sin\ \omega t$, and its general solution is

$$\boxed{x=c_1\cos\omega t+c_2\sin\omega t}$$

This expression can also be written as

$$\begin{cases} Here\ \ \mathrm{x}=c_1\cos\omega t+c_2\sin\omega t \\ Let\ \mathrm{c}_1=a\cos\alpha \ \ \text{and}\ c_2=-a\sin\alpha \\ x=a\cos\alpha\cos\omega t-a\sin\alpha\sin\omega t \\ =a\cos(\omega t+\alpha) \end{cases}$$

$$\boxed{x=a\cos(\omega t+\alpha)}$$

Where $a=\sqrt{c_1^2+c_2^2}$, $\tan\alpha=-\frac{c_2}{c_1}$

$$\dot{x}=-a\omega\sin(\omega t+\alpha)$$

The energy of a system executing small oscillations is E=T+U

$$\boxed{E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2}$$

$$E = \frac{1}{2}m\left[-a\omega\sin(\omega t+\alpha)\right]^2 + \frac{1}{2}m\omega^2\left[a\cos(\omega t+\alpha)\right]^2$$

$$= \frac{1}{2}ma^2\omega^2\left[\sin^2(\omega t+\alpha)+\cos^2(\omega t+\alpha)\right]$$

$$\boxed{E = \frac{1}{2}m\omega^2a^2}$$

The time dependence of the coordinate of an oscillating system is often conveniently represented as the real part of a complex expression :

$$x = a\cos(\omega t+\alpha)$$

$$x = Re\ a\exp i\ (\omega t+\ \alpha)$$

$$x = Re[a\ expi\alpha.\ expi\omega t]$$

$$\boxed{x = Re[A\exp(i\omega t)]\ \text{ where } A = a\exp i\alpha}$$

where A is a complex constant and it is called the complex amplitude and its argument α is initial phase.

Example 5.1 Determine the form of a curve such that the frequency of oscillations of a particle on it under the force of gravity is independent of amplitude.

Sol. Similar case we know about one dimensional simple harmonic oscillator in which $T = \frac{1}{2}\ m\ \dot{x}^2\ \ , U = \frac{1}{2}k\ x^2$ and frequency of oscillation $\omega\ = \sqrt{k/m}$ which is independent of amplitude.)

For the problem given in question ,curve satisfying the given condition(frequency of oscillation is independent of frequency) is one for which the P.E. of a particle moving on it is in form $U = \frac{1}{2}k\ s^2$ where s is the length of arc from the position of equilibrium. The kinetic energy is $T = \frac{1}{2}\ m\ \dot{s}^2$

$Angular\ frequency\ \omega\ = \sqrt{k/m}$ whatever the initial value of S.

Particle has potential energy due to gravity only that is U=mgy where y is the vertical coordinate. So this U must be in form of $\frac{1}{2}ks^2$

$\therefore \frac{1}{2}ks^2 = mgy \quad or \quad \therefore y = \frac{1}{2}\frac{k}{mg}s^2$

$y = \frac{\omega^2 s^2}{2g}$ where $\omega = \sqrt{k/m}$

For path we have to eliminate s

For arc element $ds^2 = dx^2 + dy^2$

or $dx^2 = ds^2 - dy^2$ or $dx = \left\{\left(\frac{ds}{dy}\right)^2 - 1\right\}^{\frac{1}{2}} dy$ (1)

$$y = \frac{\omega^2 s^2}{2g} \quad or \quad \frac{dy}{ds} = \frac{\omega^2 . 2s}{2g} = \frac{\omega^2}{g}\left(\frac{2gy}{\omega^2}\right)^{\frac{1}{2}}$$

Putting the value of $\frac{dy}{ds}$ in eq.(1)and integrating

$$x = \int \left(\frac{g}{2w^2 y} - 1\right)^{\frac{1}{2}} dy$$

Let $\alpha = \frac{g}{\omega^2}$ We get

$$x = \int\left(\frac{\alpha}{y} - 1\right)^{\frac{1}{2}} dy$$

For solving this integral ,assume

$y = \alpha \sin^2\theta$

or $dy = 2\alpha \sin\theta\cos\theta\, d\theta$

therefore

$$x = \int \left(\cos ec^2\theta - 1\right)^{\frac{1}{2}} 2\alpha \sin\theta\cos\theta\, d\theta$$

$$= 2\alpha\int \cot\theta \sin\theta\cos\theta\, d\theta = 2\alpha\int \sin^2\theta\, d\theta$$

$$= 2\alpha\int\left(\frac{1-\cos 2\theta}{2}\right)d\theta = \alpha\left[\theta - \frac{\sin 2\theta}{2}\right]$$

$$= \frac{\alpha}{2}\left(2\theta - \sin 2\theta\right)$$

Let $2\theta = \varepsilon$, *Then* $x = \frac{\alpha}{2}\left(\varepsilon - \sin\varepsilon\right)$

We can write $y = \alpha \sin^2\theta = \frac{\alpha}{2}(1-\cos 2\theta)$

$$y = \frac{\alpha}{2}(1-\cos\varepsilon) \quad \because 2\theta = \varepsilon$$

Thus $\boxed{x = \frac{\alpha}{2}(\varepsilon - \sin\varepsilon) \quad \text{and} \quad y = \frac{\alpha}{2}(1-\cos\varepsilon)}$

These are equations of the required curve (*Cycloid*) in parametric form.

5.3 Forced Oscillations

Let us now consider oscillations of a system on which a variable external force acts. These are called 'forced' oscillations.

Since the oscillations are again supposed small, it is implied that the external field is weak, otherwise it would cause displacement x to take too large values.

The system now has besides the potential energy $P.E. = \frac{1}{2}kx^2$, the additional potential energy $U_e(x,t)$ resulting from the external field. In general $U_e(x,t)$ is function of displacement x and time t .In absence of external field, equilibrium position was $x = 0$

Now expanding $U_e(x,t)$ about $x = 0$,then by Taylor's series

$$U_e(x,t) = U_e(0,t) + x \left.\frac{\partial U_e}{\partial x}\right|_{x=0} + \cdots$$

The first term $U_e(0,t) = [U_e(0,t)]_{x=0}$ is a function of time only and may therefore be omitted from the Lagrangian.

In the second term $-\left[\frac{\partial U_e}{\partial x}\right]_{x=0}$ is the external 'force' acting on the system in the equilibrium position and is a given function of time which we denote by $F(t)$.

Thus the potential energy involves a further term $- x F(t)$

So we have $U_e(x,t) = U_e(0,t) - x F(t)$

We have neglected the higher order terms.

Since $\frac{d}{dt}\left(\frac{\partial}{\partial \dot{x}}U_e(0,t)\right) - \frac{\partial}{\partial x}U_e(0,t) = 0 - 0 = 0$

So the term $U_e(0,t)$ may be omitted from the Lagrangian .

We can write Lagrangian of the system as

L=T−U or

$$L = \frac{1}{2} m \dot{x}^2 - \left[\frac{1}{2} kx^2 - x F(t)\right] \quad (1)$$

The corresponding equation of motion is :

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \Rightarrow \frac{d}{dt}\left(\frac{1}{2} m 2\dot{x}\right) - \left[-\left(\frac{1}{2} k 2x - F(t)\right)\right] = 0$$

$$m\ddot{x} + kx = F(t)$$

$$or \quad \ddot{x} + \omega^2 x = \frac{F(t)}{m} \quad (2)$$

where $\omega = \sqrt{k/m}$

The general solution of this inhomogeneous linear differential equation is with constant coefficient is $x = x_0 + x_1$

Where x_0 is solution of the corresponding homogenous equation and x_1 is a particular integral of the inhomogenous equatuion.

If we take special case in which

$$\text{Let } F(t) = f\cos(\gamma t + \beta) \quad (3)$$

Here f, γ, β are constants. γ is the frequency of the external source.

Now eq. (2) becomes $\ddot{x} + \omega^2 x = \frac{f}{m}\cos(\gamma t + \beta)$

By differential equations, We seek a particular integral of equation (2) in the form $x_1 = b\cos(\gamma t + \beta)$ with the same periodic factor.

Substituting x_1 in that equation, we get

$$\ddot{x}_1 + \omega^2 \ddot{x}_1 = \frac{f}{m}\cos(\gamma t + \beta)$$

$$-b\gamma^2 \cos(\gamma t + \beta) + -b\omega^2 \cos(\gamma t + \beta) = \frac{f}{m}\cos(\gamma t + \beta)$$

$$\Rightarrow -b\gamma^2 - b\omega^2 = \frac{f}{m}$$

$$\Rightarrow b = \frac{f}{m\left(\omega^2 - \gamma^2\right)}$$

$$\therefore x_1 = b\cos(\gamma t + \beta) = \frac{f}{m\left(\omega^2 - \gamma^2\right)}\cos(\gamma t + \beta)$$

Adding the solution of the homogenous equation(2), we obtain the general integral in the form :

$$x = x_0 + x_1$$

$$x = a\cos(\omega t + \alpha) + \frac{f}{m(\omega^2 - \gamma^2)}\cos(\gamma t + \beta) \qquad (4)$$

The arbitrary constants a and α are found from the initial conditions.

Eq. (4) is not valid when resonance occurs i.e. when the frequency γ of the external force is equal to the intrinsic frequency ω of the system.

To find the general solution of the equation of motion in this case we rewrite (4) as

$$x = a'\cos(\omega t + \alpha) + \left[\frac{f}{m(\omega^2 - \gamma^2)}\{\cos(\gamma t + \beta) - \cos(\omega t + \beta)\}\right] \text{ Where } a' \neq a \text{ As}$$

$\gamma \to \omega$ the second term is indeterminate of the form $\frac{0}{0}$. Resolving the indeterminacy by L' Hospital's rule.

$$Here \quad \text{Lim } \gamma \to \omega \quad \frac{f\{(\cos(\gamma t + \beta) - \cos(\omega t + \beta)\}}{m(\omega^2 - \gamma^2)}$$

$$= \text{Lim } \gamma \to \omega \quad \frac{\frac{d}{d\gamma}\frac{f}{m}\{(\cos(\gamma t + \beta) - \cos(\omega t + \beta)\}}{\frac{d}{d\gamma}(\omega^2 - \gamma^2)}$$

$$= \text{Lim}\gamma \to \omega \quad \frac{\frac{f}{m}\{-t\sin(\gamma t + \beta) - 0\}}{0 - 2\gamma}$$

$$= \frac{ft\sin(\omega t + \beta)}{2m\gamma}$$

$$x = a'\cos(\omega t + \alpha) + \frac{ft}{2m\omega}\sin(\omega t + \beta)$$

Thus the amplitude in resonance increases linearly only with time until the oscillations are no longer small and the whole theory given above becomes invalid.

Let us also ascertain the nature of small oscillations near resonance, when $\gamma = \omega + \varepsilon$ with ε a small quantity. We put the general solution in the complex form :

$$x = x_0 + x_1 = a\cos(\omega t + \alpha) + b\cos(\gamma t + \beta)$$

$$= \mathrm{Re}\left[a\exp i(\omega t + \alpha) + b\exp i(\gamma t + \beta)\right]$$

$$= \mathrm{Re}\left[\left(a\exp i\alpha\right)\exp i\omega t + (b\exp i\beta)\exp i\gamma t\right]$$

$$= \mathrm{Re}\left[A\exp i\omega t + B\exp i\gamma t\right] \text{ where } A = \left(a\exp i\alpha\right) and\ B = (b\exp i\beta)$$

$$= \mathrm{Re}\left[A\exp i\omega t + B\exp i(\omega t + \varepsilon t)\right]$$

$$= \mathrm{Re}\left[(A + B\exp i\varepsilon t)\exp i\omega t\right]$$

$$= \mathrm{Re}\left[C\exp i\omega t\right]$$

Where $C = A + B\exp i\varepsilon t$

$$C = a\exp i\alpha + b\exp i\beta\exp i\varepsilon t$$

$$= a\exp i\alpha + b\exp i(\beta + \varepsilon t)$$

$$|C|^2 = CC^* = \left[a\exp i\alpha + b\exp i(\beta + \varepsilon t)\right]\left[a\exp(-i\alpha) + b\exp\{-i(\beta + \varepsilon t)\}\right]$$

$$|C|^2 = a\exp(i\alpha)\ a\exp(-i\alpha) + a\exp(i\alpha)\ b\exp\{-i(\beta + \varepsilon t)\}$$
$$+ b\exp i(\beta + \varepsilon t)\ a\exp(-i\alpha) + b\exp i(\beta + \varepsilon t)\ b\exp\{-i(\beta + \varepsilon t)\}$$

$$|C|^2 = a^2 + b^2 + ab[\exp i(\alpha - \beta + \varepsilon t) + \exp - i(\alpha - \beta + \varepsilon t)]$$

$$|C|^2 = a^2 + b^2 + 2ab\cos(\alpha - \beta + \varepsilon t)$$

$If\ \cos(\alpha - \beta + \varepsilon t) = 1, then\ |C|^2 = (a + b)^2$

$If\ \cos(\alpha - \beta + \varepsilon t) = -1, then |C|^2 = (a - b)^2$

Since the quantity $C = A + B\ exp\ (i\varepsilon t)$ varies only slightly over the period $\frac{2\pi}{\omega}$ of the factor $exp\ (i\omega t)$, the motion near resonance may be regarded as small oscillations of variable amplitude. Denoting the amplitude by C

Thus the amplitude varies periodically with freq. ε between the limits $|a - b| \leq C \leq (a + b)$. This phenomenon is called beats.

The equation of motion $\ddot{x} + \omega^2 x = \frac{F(t)}{m}$ can be integrated in a general form for an arbitrary external force (t). :

Rewriting the equation $\ddot{x} + \omega^2 x = \frac{F(t)}{m}$ as

$$\ddot{x} + i\omega\dot{x} - i\omega\dot{x} - i^2\omega^2 x = \frac{F(t)}{m}$$

Or $\frac{d}{dt}(\dot{x}+i\omega x)-i\omega(\dot{x}+i\omega x)=\frac{1}{m}F(t)$

Let $\xi=\dot{x}+i\omega x$

Then above equation becomes $\frac{d\xi}{dt}-i\omega\xi=\frac{F(t)}{m}$ (1)

For solution of above nonhomogeneous equation we assume,

$$\xi=A(t)e^{i\omega t} \tag{2}$$

Putting this $\xi=A(t)e^{i\omega t}$ in eq.(1) ,we get

$$\frac{d}{dt}\left(A(t)e^{i\omega t}\right)-i\omega\left(A(t)e^{i\omega t}\right)=\frac{F(t)}{m}$$

$$e^{i\omega t}\frac{dA}{dt}+i\omega e^{i\omega t}A-i\omega e^{i\omega t}A=\frac{F}{m}$$

$$\frac{dA}{dt}=\frac{F}{m}e^{-i\omega t}\Rightarrow\quad dA=\frac{F}{m}e^{-i\omega t}dt$$

$$\int dA=\int\frac{F}{m}e^{-i\omega t}dt \tag{3}$$

$$A(t)-A(0)=\int_0^t\frac{F(t)}{m}e^{-i\omega t}dt\Rightarrow A(t)=\int_0^t\frac{F(t)}{m}e^{-i\omega t}dt+A(0)$$

$$From\,(2)\,\xi=e^{i\omega t}\left\{\int_0^t\frac{F(t)}{m}e^{-i\omega t}dt+A(0)\right\}$$

Putting $t=0$ $in\,\xi=A(t)e^{i\omega t}$ $We\,have\,\xi(0)=A(0)e^{i\omega 0}=A(0)$

Thus $\xi=e^{i\omega t}\left\{\int_0^t\frac{F(t)}{m}e^{-i\omega t}dt+\xi(0)\right\}$

We have assumed $\xi=\dot{x}+i\omega x$ Since x is real function of time ,imaginary part of ξ is given by ωx .Thus function $x(t)$ is given by the imaginary part ξ divided by ω.

The energy of the system is

$$E=\frac{1}{2}m\dot{x}^2+\frac{1}{2}kx^2=\frac{1}{2}m\dot{x}^2+\frac{1}{2}m\omega^2x^2=\frac{1}{2}m(\dot{x}^2+\omega^2x^2)$$

$$Here\,\xi=\dot{x}+i\omega x,\xi^*=\dot{x}-i\omega x\quad or\,\xi\xi^*=\dot{x}^2-(i\omega x)^2=\dot{x}^2+\omega^2x^2=|\xi|^2$$

$$So\,E=\frac{1}{2}m|\xi|^2$$

Above system is example of forced oscillations in which energy of system is not conserved, because system gains energy from the external source. We now determine the total energy transmitted to the system during all time, assuming its initial energy to be zero.

$$From\, eq.(3) \int dA = \int \frac{F}{m} e^{-i\omega t} dt$$

$$or\ A(t) - A(t_1) = \int_{t_1}^{t} \frac{F}{m} e^{-i\omega t} dt$$

$$A(t) = \int_{t_1}^{t} \frac{F}{m} e^{-i\omega t} dt + A(t_1)$$

$$Thus\, \xi(t) = e^{i\omega t} \left\{ \int_{t_1}^{t} \frac{F(t)}{m} e^{-i\omega t} dt + A\left(t_1\right) \right\}$$

$$\xi(t) = e^{i\omega t} A\left(t_1\right) + \int_{t_1}^{t} \frac{F(t)}{m} e^{-i\omega t} dt$$

$$\xi(t) = \xi\left(t_1\right) + \int_{t_1}^{t} \frac{F(t)}{m} e^{-i\omega t} dt$$

$$\because \xi = A(t) e^{i\omega t}$$

$$\xi(t) = \xi\left(-\infty\right) + \int_{-\infty}^{t} \frac{F(t)}{m} e^{-i\omega t} dt$$

$$With\, \xi\left(-\infty\right) = 0,\ \text{above expression} \xi(t) = \int_{-\infty}^{t} \frac{F(t)}{m} e^{-i\omega t} dt$$

$$For\, t \to \infty,\ \xi(\infty) = \frac{1}{m} \int_{-\infty}^{\infty} F(t) e^{-i\omega t} dt$$

$$\left|\xi(\infty)\right|^2 = \frac{1}{m^2} \left| \int_{-\infty}^{\infty} F(t) e^{-i\omega t} dt \right|^2$$

Substituting $\left|\xi(\infty)\right|^2$ obtain the energy transferred $E = \frac{1}{2} m \left|\xi\right|^2$:

$$E = \frac{1}{2m} \left| \int_{-\infty}^{\infty} F(t) \exp(-i\omega t) dt \right|^2$$

From above expression we can conclude that the energy is determined by the squared modulus of the Fourier component of the force $F(t)$ whose frequency

is the intrinsic frequency of the system.

In particular, if the external force acts only during a time short in comparison with $\frac{1}{\omega}$, i.e. $\omega t \ll 1$ we can put $\exp(-i\omega t) \approx 1$.

Then $E = \frac{1}{2m}\left(\int_{-\infty}^{\infty} F(t)dt\right)^2$

If we compare with expression $E = \frac{P^2}{2m}$,then it expresses the fact that a force of short duration gives the system a momentum $\int Fdt$ without bringing about a perceptible displacement.

5.4 Oscillations of Systems With More than One Degree of Freedom

In the following we give the theory of force oscillations of systems with s degrees of freedom.

Let the potential energy of the system U as a function of the generalized coordinates q_i $(i = 1, 2, \ldots . s)$ have a minimum for $q_i = q_{io}$.

Putting deviation of coordinates from equilibrium position

$$x_i = q_i - q_{i0} \qquad (1)$$

Expanding U by Taylor's series

$$U(q_1, q_2, \ldots q_i, \ldots q_s) = U(q_{1o}, q_{2o}, \ldots q_{io}, \ldots q_{so}) + \sum_i \left(\frac{\partial U}{\partial q_i}\right)_o (q_i - q_{i0})$$

$$+ \frac{1}{2}\sum_{ik}\left(\frac{\partial^2 U}{\partial q_i \partial q_k}\right)_o (q_i - q_{i0})(q_k - q_{k0}) + \ldots$$

subscript *0* denotes generalized coordinate at equilibrium position.

Where we again take the minimum value of the potential energy as zero i.e. $U(q_{1o}, q_{2o}, \ldots q_{io}, \ldots q_{so}) = 0$

Generalized forces evaluated at the position of equilibrium must vanish i.e. $\left(\frac{\partial U}{\partial q_i}\right)_o = 0$

Thus above expression becomes

$$U=0+0+\frac{1}{2}\sum_{ik}\left(\frac{\partial^2 U}{\partial q_i \partial q_k}\right)_o (q_i - q_{i0})(q_k - q_{k0})$$

$$U=\frac{1}{2}\sum_{ik} k_{ik} x_i x_k \quad \text{Where } x_i = q_i - q_{i0} \text{ and } x_k = q_k - q_{k0} \text{ and}$$

$$k_{ik} = \left(\frac{\partial^2 U}{\partial q_i \partial q_k}\right)_o = \left(\frac{\partial^2 U}{\partial q_k \partial q_i}\right)_o = k_{ki}$$

and U as a function of x_i as far as the quadratic terms,

$$\boxed{U = \frac{1}{2}\sum_{i,k} k_{ik} x_i x_k} \tag{2}$$

In the kinetic energy, which has the general form $\boxed{T = \frac{1}{2}\sum_{i,k} a_{ik}(q)\dot{q}_i \dot{q}_k}$ we put $q_i = q_{io}$ in the coefficients a_{ik} then to a good approximation $a_{ik}(q)$ can be taken to be their value at the position of stable equilibrium i.e. $a_{ik}(q) \cong a_{ik}(q_0)$ where $q_o = (q_{1o}, q_{2o}, \ldots q_{io}, \ldots q_{so})$ and, denoting $a_{ik}(q_0)$ by m_{ik} ,we obtain the kinetic energy as a positive definite quadratic form:

$$\boxed{T = \frac{1}{2}\sum_{i,k} m_{ik} \dot{x}_i \dot{x}_k} \tag{3}$$

Obviously by symmetry $m_{ik} = m_{ki}$

Thus the Lagrangian of a system executing small force oscillations

$$L = T - U = \frac{1}{2}\sum_{i,k}(m_{ik}\ \dot{x}_i\ \dot{x}_k\ - \frac{1}{2}\sum_{i,k} k_{ik}\ x_i\ x_k$$

$$L = \tfrac{1}{2}\textstyle\sum_{i,k}(m_{ik}\ \dot{x}_i\ \dot{x}_k\ - k_{ik}\ x_i\ x_k\ ) \tag{4}$$

Let us now derive the equations of motion. To determine the derivatives involved, we write the total differential of the Lagrangian.

$$dL = \frac{1}{2}\sum_{i,k}\{m_{ik}\ \dot{x}_i\ d\dot{x}_k + m_{ik}\ \dot{x}_k\ d\dot{x}_i\ - k_{ik}\ x_i\ dx_k - k_{ik}\ x_k\ dx_i\}$$

Since the value of the sum is obviously independent of the naming of the suffixes, we can interchange i and k in the first and third terms in the parentheses using the symmetry of m_{ik} and k_{ik} we have$m_{ik} = m_{ki}$, $k_{ik} = k_{ki}$
and

$$dL = \frac{1}{2}\sum_{i,k}\left\{m_{ki}\ \dot{x}_k\ d\dot{x}_i + m_{ki}\ \dot{x}_k\ d\dot{x}_i \quad - k_{ik}\ x_k\ dx_i - k_{ik}\ x_k\ dx_i\right\}$$

$$dL = \sum (m_{ik}\ \dot{x}_k\ d\dot{x}_i\ - k_{ik}\ x_k\ dx_i)$$

We know that

$$dL = \sum\ \left(\frac{\partial L}{\partial \dot{x}_i} d\dot{x}_i + \frac{\partial L}{\partial x_i} dx_i\right)$$

Hence by comparison of above terms ,we have

$$\frac{\partial L}{\partial \dot{x}_i} = \sum_k m_{ik}\ \dot{x}_k$$

$$\frac{\partial L}{\partial x_i} = -\sum_k k_{ik}\ x_k$$

Lagrange's equations are therefore $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0$

$$\sum_k m_{ik}\ \ddot{x}_k + \sum_k k_{ik}\ x_k = 0 \qquad (i = 1, 2, \ldots . s) \tag{5}$$

They form a set of s linear homogenous differential equations with constant coefficients.

As usual, we seek the s unknown functions $x_k(t)$ in the form :

$$x_k = A_k \exp\ (i\omega t) \tag{6}$$

Where A_k are in general some complex constant to be determined. Substituting (6) in (5) and cancelling $\exp(i\omega t)$, we obtain a set of linear homogenous algebraic equations to be satisfied by the A_k :

$$\sum_k m_{ik} A_k (i\omega)^2 expi\omega t + \sum_k k_{ik} A_k expi\omega t\ = 0$$

$$\sum_k (-\omega^2 m_{ik} + k_{ik})\ A_k = 0 \tag{7}$$

If this system has non-zero solutions, the determinant of the coefficients must vanish:

$$|k_{ik} - \omega^2 m_{ik}| = 0 \tag{8}$$

This is the characteristic equation and is of degree s in ω^2. In general, it has s different real positive roots ω_α^2 $(\alpha = 1, 2, \ldots., s)$; in particular cases, some of these roots may coincide.

These quantities ω_α are the characteristic frequencies or eigen frequencies of the system.

It is evident from physical arguments that the roots of eq. (8) are real and positive. For the existence of an imaginary part of ω would mean the presence, in the time dependence of the coordinates

$x_k\left[viz. x_k = A_k\, e^{i\omega t}\ let\ \omega = (\gamma + i\beta)\ x_k = A_k\, e^{i\gamma t} e^{-\beta t}\right]$ and so of the velocities $\dot{x}_k$ of an exponentially decreasing or increasing factor. Such a factor is inadmissible, since it would lead to a time variation of total energy $E = U + T$ of the system, which would therefore not be conserved.

The frequencies ω_α having been found, we substitute each of them in (7) and find the corresponding coefficients A_k.

If all the roots ω_α of the characteristic equation are different, the coefficients A_k are proportional to minors of the determinant (8) and with $\omega = \omega_\alpha$.

Let these minors be $\Delta_{k\alpha}$.

A particular solution of the differential equation (5) is therefore $x_k = \Delta_{k\alpha} C_\alpha \exp\ (i\ \omega_\alpha t)$, where C_α is an arbitrary complex constant.

The general solution is the sum of s particular solutions. Taking the real part we have

$$x_k = Re \sum_{\alpha=1}^{s} \Delta_{k\alpha} C_\alpha \exp(i\omega_\alpha t)$$

$$= \sum \Delta_{k\alpha}\, \varkappa_\alpha \qquad (9)$$

Where $\varkappa_\alpha = Re[C_\alpha \exp(i\omega_\alpha t)]$ (10)

Thus the time variation of each coordinate of the system is a superposition of s simple periodic oscillations $\varkappa_1, \varkappa_2, \ldots\ldots \varkappa_s$ with arbitrary amplitudes and phases but definite frequencies.

The question arises whether the generalized coordinates can be chosen in such a way that each of them executes only one simple oscillation.

The form of the general solution (9) points to the answer .For regarding the *s* equations (9) as a set of equations for *s* unknowns $\varkappa_\alpha$ we can express $\varkappa_1 , \varkappa_2 , \ldots\ldots \varkappa_s$ in terms of the coordinates $x_1 , \ldots\ldots x_s$.

The quantities $\varkappa_\alpha$ may therefore be regarded as new generalized coordinates, called normal coordinates and they execute simple periodic oscillations called normal oscillations of the system.

The normal coordinates $\varkappa_\alpha$ are seen from their definition to satisfy the following equations :

$$\ddot{\varkappa}_\alpha + \omega_\alpha^2 \varkappa_\alpha = 0 \qquad (11)$$

This mean that in normal coordinates the equations of motion become *s* independent equations.

It is evident that the Lagrangian expressed in terms of normal coordinates is of the form :

$$L = \sum_\alpha \frac{1}{2} m_\alpha (\dot{\varkappa}_\alpha^2 - \omega_\alpha^2 \varkappa_\alpha^2) \qquad (12)$$

Since with this form of L, by using $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\varkappa}_\alpha}\right) - \frac{\partial L}{\partial \varkappa_\alpha} = 0$ we can get $\ddot{\varkappa}_\alpha + \omega_\alpha^2 \varkappa_\alpha = 0$

Mathematically, this means that the transformation (9) simultaneously puts both quadratic forms – the kinetic energy (3) and the potential energy (2) in the diagonal form.

The normal coordinates are usually chosen so as to make the coefficients of the squared velocities in the Lagrangian equal to one-half. This can be achieved by simply defining now normal coordinates .

$$Q_\alpha = \sqrt{m_\alpha}\ \varkappa_\alpha.$$

Then by using (12) $L = \frac{1}{2}\sum_\alpha \left[\left(\sqrt{m_\alpha}\ \dot{\varkappa}_\alpha\right)^2 - \omega_\alpha^2\left(\sqrt{m_\alpha}\ \varkappa_\alpha\right)^2\right]$

$$L = \frac{1}{2}\sum_\alpha \left(\dot{Q}_\alpha^2 - \omega_\alpha^2 Q_\alpha^2\right)$$

The above discussion needs little alternation when some roots of the characteristic equation coincide. In this case the coefficient Δ corresponding to multiple roots are not the minors of the determinant, which in this case vanish. Each multiple (or, as we say degenerate) frequency corresponds to a number of normal coordinates equal to its multiplicity but choice of these coordinates is not unique.

Example 5.2 Find the normal coordinates and eigen frequencies of a three dimensional oscillator having potential energy

$$U = \frac{1}{2}\,(k_1x^2 + k_2y^2 + k_3z^2)$$

Sol.

$$\boxed{\begin{aligned} T &= \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) \\ U &= \frac{1}{2}\left(k_1x^2 + k_2y^2 + k_3z^2\right) \end{aligned}}$$

$$\therefore\ L = \frac{1}{2}\,m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \frac{1}{2}\,(k_1x^2 + k_2y^2 + k_3z^2)$$

$$= \frac{1}{2}\,m(\dot{x}^2 - \omega_1^2x^2) + \frac{1}{2}\,m(\dot{y}^2 - \omega_2^2y^2) + \frac{1}{2}m(\dot{z}^2 - \omega_3^2z^2$$

$$Where\ \omega_1 = \sqrt{\frac{k_1}{m}}\ ,\qquad \omega_2 = \sqrt{\frac{k_2}{m}}\ ,\qquad \omega_3 = \sqrt{\frac{k_3}{m}}$$

By Lagrange's equation of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0 \quad \text{or} \quad \frac{d}{dt}\,(m\dot{x}) - (-m\omega_1^2x) = 0$$

$$\ddot{x} + \omega_1^2x = 0 \quad \text{or } x = Acos(\omega_1t + \alpha)$$

Here x is referred as the normal coordinate because equation of motion in it contain a single frequency ω_1

Similarly we can get $\ddot{y} + \omega_2^2y = 0$ and y is normal coordinate.

Similarly $\ddot{z} + \omega_3^2z = 0$ and z is normal coordinate

Thus Normal coordinates are x, y, z and eigenfrequencies are $\omega_1, \omega_2, \omega_3$.

Note that in case of ***central field*** $\boldsymbol{k_1 = k_2 = k_3}$, $\boldsymbol{U = \frac{1}{2}kr^2}$. The three frequencies are equal.

Example 5.3 Determine the oscillations of a system with two degrees of freedom whose Lagrangian is :

$$L = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) - \tfrac{1}{2}\,\omega_0^2\,(x^2 + y^2) + \,\alpha xy$$

(two identical one-dimensional systems of eigenfrequency ω_0 coupled by an interaction $-\alpha xy$.

Sol. $L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}\omega_0^2 (x^2 + y^2) + \alpha xy$

Lagranges equation of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$$

$$\frac{d}{dt}(\dot{x}) - (-\omega_0^2 x + \alpha y) = 0$$

$$or\ \ddot{x} + \omega_0^2 x = \alpha y \qquad (1)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) - \frac{\partial L}{\partial y} = 0$$

$$and\ \ddot{y} + \omega_0^2 y = \alpha x \qquad (2)$$

$Let\ x = A_x \exp(i\omega t), y = A_y \exp(i\omega t),$

Where A_x and A_y are complex amplitudes, putting these values in eqn. (1) and (2)

$$A_x(i\omega)^2 \exp(i\omega t) + \omega_0^2 A_x \exp(i\omega t) = \alpha A_y \exp(i\omega t)$$

$$(\omega_0^2 - \omega^2) A_x - \alpha A_y = 0 \qquad (3)$$

$From\,(2)$

$$A_y(i\omega)^2 \exp(i\omega t) + \omega_0^2 A_y \exp(i\omega t) = \alpha A_x \exp(i\omega t)$$

$$\alpha A_x - (\omega_0^2 - \omega^2) A_y = 0 \qquad (4)$$

From (3) and (4),the characteristic equation is $\begin{vmatrix} \omega_0^2 - \omega^2 & -\alpha \\ \alpha & -(\omega_0^2 - \omega^2) \end{vmatrix} = 0$

$$or\quad -(\omega_0^2 - \omega^2)^2 + \alpha^2 = 0$$

$$(\omega_0^2 - \omega^2)^2 = \alpha^2$$

$$\omega_0^2 - \omega^2 = \pm\alpha$$

Case(I) $\omega = \omega_1\ then\ \omega_0^2 - \omega_1^2 = \alpha$

$$or\ \ \omega_1^2 = \omega_0^2 - \alpha$$

Case(II) $\omega = \omega_2\ \ then\ \omega_0^2 - \omega_2^2 = -\alpha$

$$or\ \ \omega_2^2 = \omega_0^2 + \alpha$$

Case (I)

$\omega = \omega_1$ putting the value $\omega_1^2 = \omega_0^2 - \alpha$ in eq. (3) or (4) we get

$$(\omega_0^2 - \omega_1^2) A_{x1} - \alpha A_{y1} = 0$$

$$\alpha A_{x1} - \alpha A_{y1} = 0 \text{ or } A_{x1} = A_{y1} \qquad (5)$$

$\because x = A_x \exp(i\omega t)$ *and* $y = A_y \exp(i\omega t)$

$\therefore x = A_{x1} \exp(i\omega_1 t)$ and $y = A_{y1} \exp(i\omega_1 t) = A_{x1} \exp(i\omega_1 t)$ (6)

Case(II)

$\omega = \omega_2$ putting the value $\omega_2^2 = \omega_0^2 + \alpha$ in eq. (3) or (4) we get

$(\omega_0^2 - \omega_2^2) A_{x2} - \alpha A_{y2} = 0$

$-\alpha A_{x2} - \alpha A_{y2} = 0$ or $A_{x2} = -A_{y2}$ (7)

$\because x = A_x \exp(i\omega t)$ *and* $y = A_y \exp(i\omega t)$

$\therefore x = A_{x2} \exp(i\omega_2 t)$ and $y = A_{y2} \exp(i\omega_2 t) = -A_{x2} \exp(i\omega_2 t)$ (8)

If system is excited arbitrarily it will not respond with a single mode of oscillation but in general with a mixture of all possible modes in each coordinates. From(6)and(7),general solution is given by

$x = A_{x1} \exp(i\omega_1 t) + A_{x2} \exp(i\omega_2 t)$

$y = A_{x1} \exp(i\omega_1 t) - A_{x2} \exp(i\omega_2 t)$

If we assume $x = c(Q_1 + Q_2)$ and $y = c(Q_1 - Q_2)$

Putting these values in the Lagrangian

$$L = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) - \tfrac{1}{2}\,\omega_0^2\,(x^2 + y^2) + \alpha xy$$

$$L = \frac{1}{2}c^2\left(\dot{Q}_1^2 + \dot{Q}_2^2 + 2\dot{Q}_1\dot{Q}_2 + \dot{Q}_1^2 + \dot{Q}_2^2 - 2\dot{Q}_1\dot{Q}_2\right)$$

$$-\frac{\omega_0^2}{2}c^2\left(Q_1^2 + Q_2^2 + 2Q_1Q_2 + Q_1^2 + Q_2^2 - 2Q_1Q_2\right) + \alpha c^2(Q_1^2 - Q_2^2)$$

$$L = c^2\left(\dot{Q}_1^2 + \dot{Q}_2^2\right) - c^2\omega_0^2\left(Q_1^2 + Q_2^2\right) + \alpha c^2(Q_1^2 - Q_2^2)$$

$$L = c^2\left[\left\{\dot{Q}_1^2 - (\omega_0^2 - \alpha)Q_1^2\right\} + \left\{\dot{Q}_2^2 - (\omega_0^2 + \alpha)Q_2^2\right\}\right]$$

$$L = c^2\left[\left\{\dot{Q}_1^2 - \omega_1^2 Q_1^2\right\} + \left\{\dot{Q}_2^2 - \omega_2^2 Q_2^2\right\}\right]$$

$$L = c^2 \sum_n \left\{\dot{Q}_n^2 - \omega_n^2 Q_n^2\right\}$$

We know that ***standard form of Lagrangian for normal coordinates*** is

$$\boldsymbol{L = \frac{1}{2}\sum_n \left\{\dot{Q}_n^2 - \omega_n^2 Q_n^2\right\}}$$

By comparison we can say $c = \frac{1}{\sqrt{2}}$

Thus oscillation frequency for normal coordinate Q_1 is ω_1 and for normal coordinate Q_2 is ω_2 .In terms of normal coordinates Q_1 and Q_2 ,generalized coordinates x,y are given as

$$x = c(Q_1 + Q_2) = \frac{1}{\sqrt{2}}(Q_1 + Q_2) \text{ and } y = c(Q_1 - Q_2) = \frac{1}{\sqrt{2}}(Q_1 - Q_2)$$

If there is no interaction term αxy in Lagrangian , then Lagrangian becomes $L = \frac{1}{2}[(\dot{x}^2 + \dot{y}^2) - \omega_0^2 (x^2 + y^2)]$ and frequency of oscillation would be ω_0 .Due to interaction term we got two different values of oscillation frequency ω i.e. $\omega_1 = \sqrt{\omega_o^2 - \alpha}$ and $\omega_2 = \sqrt{\omega_o^2 + \alpha}$

If coupling is weak i.e. $\alpha \ll \omega_0^2$

then $\omega_1^2 = \omega_0^2 - \alpha$

$$= \omega_0 \left(1 - \frac{\alpha}{\omega_0^2}\right)^{\frac{1}{2}} \qquad \therefore \ \omega_1 \approx \omega_0 \left(1 - \frac{1}{2}\frac{\alpha}{\omega_0^2}\right)$$

$$\approx \omega_0 - \frac{\alpha}{2\omega_0}$$

And similarly $\omega_2 = \sqrt{\omega_o^2 + \alpha}$ becomes $\omega_2 = \omega_0 + \frac{\alpha}{2\omega_0}$

Since $\frac{\alpha}{\omega_0} << \omega_0$ We have $\omega_1 \approx \omega_2$

The variation of x and y in this case is a superposition of two oscillations with almost equal frequencies i.e. beats of frequency

$\omega_2 - \omega_1 \approx \left(\omega_0 + \frac{\alpha}{2\omega_0}\right) - \left(\omega_0 - \frac{\alpha}{2\omega_0}\right) = \frac{\alpha}{\omega_0}$ The amplitude of y is a minimum when that of x is a maximum and vice-versa.

5.5 Self Learning Exercise-I

Very Short Answer Type Questions

Q.1 Find the frequency ω of oscillations of a diatomic molecule consisting of atoms of masses m_1 and m_2 having "force constant" k .

Q.2 What are normal coordinates?

Short Answer Type Questions

Q.3 Two masses m_1 and m_2 are connected by a spring of force constant k. The spring is compressed and released .Find the frequency of oscillation of the system.

Q.4 Express the amplitude and initial phase of the oscillations in terms of the initial coordinates x_0 and velocity v_0.

Example 5.4 Find the path of a particle in a central field $U = \frac{1}{2}kr^2$ (called space oscillator)

Sol. As in any central field the path lies on a plane i.e. motion of particle occurs in two dimensions, which we can take as the xy plane. Let position of particle is given by (x,y) and $r^2 = x^2 + y^2$ in two dimensional motion. Then Lagrangian L=T-U

$$L = \frac{1}{2}m\,(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}k(x^2 + y^2)$$

Lagranges equation of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$$

$$\frac{d}{dt}\,(m\dot{x}) - (-kx) = 0$$

$$\ddot{x} + \frac{k}{m}x = 0 \quad \text{or } \ddot{x} + \omega^2 x = 0$$

The variation of coordinate x is a simple oscillation with the frequency $\omega = \sqrt{\frac{k}{m}}$

General solution $x = a\cos(\omega t + \alpha)$

Similarly $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) - \frac{\partial L}{\partial y} = 0$ gives $\frac{d}{dt}\,(m\dot{y}) - (-ky) = 0$

$$\ddot{y} + \frac{k}{m}y = 0 \quad \text{or } \ddot{y} + \omega^2 y = 0 \text{ where } \omega = \sqrt{\frac{k}{m}}$$

The variation of coordinate y is a simple oscillation with the same frequency $\omega = \sqrt{\frac{k}{m}}$ General solution $y = b\cos(\omega t + \beta)$

Let $\phi = \omega t + \alpha$ then $x = a\cos\phi$,

Let $\delta = \beta - \alpha$ *then* $y = b\cos(\phi + \delta)$

$$y = b\cos\phi\cos\delta - b\sin\phi\sin\delta,$$

Putting $\cos\phi = \frac{x}{a}$ in above equation

$$y = b\frac{x}{a}\cos\delta - b\sin\phi\sin\delta$$

$$\therefore \sin\phi = \frac{y - b\frac{x}{a}\cos\delta}{-b\sin\delta}$$

For path we have to find out an expression that will be independent of time t

$$cos^2\phi + sin^2\phi = 1$$

$$\frac{x^2}{a^2} + \frac{y^2 + \frac{b^2x^2}{a^2}\,cos^2\delta - \frac{2xyb}{a}\cos\delta}{b^2sin^2\delta} = 1$$

$$\frac{x^2}{a^2}sin^2\delta + \frac{y^2}{b^2} + \frac{x^2}{a^2}cos^2\delta - \frac{2xy}{ab}\cos\delta = sin^2\delta$$

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{2xy}{ab}\cos\delta = sin^2\delta$$

5.6 Vibrations of Molecules

If we have a system of interacting particles, not in an external field, not all of its degrees of freedom relate to oscillations.

If we consider a molecule, then the atoms in it oscillate about their position of equilibrium. Besides these motions the whole molecule can execute translational and rotational motions.

A molecule containing n atoms, then of the 3 n degrees of freedom ,three degrees correspond to translational motion, and in general the same number to rotation.

So degrees of freedom of vibration is $3n - (3 + 3) = 3n - 6$.

An exception is formed ***by molecules in which atoms are collinear, for which there are only two rotational degrees of freedom (since rotation about the line of atoms is of no significance)***, and therefore vibrational degrees of freedom = $3n - (3 + 2) = 3n - 5$.

In solving mechanical problem of molecular oscillations, it is convenient to eliminate immediately the translational and rotational degrees of freedom.

Translational degrees of freedom can be removed by equating to zero the total momentum of the molecule i.e. centre of mass of the molecule is at rest, it can be

expressed by saying that the three coordinates of the centre of mass are constant. so position vector of center of mass is $\vec{r}_{cm} = \frac{\sum_a m_a \vec{r}_a}{\sum_a m_a}$ which is constant.

We have the condition:

$$\sum_a m_a \vec{r}_a = \text{constant}$$

Putting $\vec{r}_a = \vec{r}_{ao} + \vec{\varepsilon}_a$, $\vec{r}_{ao}$ is the radius vector of the equilibrium position of the a^{th} atom and $\vec{\varepsilon}_a$ is deviation.

$$\sum_a m_a \vec{r_a} = \sum_a m_a(\vec{r}_{ao} + \vec{\varepsilon}_a) = constant$$

Since displacement of center of mass is zero $\sum_a m_a \vec{\varepsilon}_a = 0$ (1)

We have $\sum_a m_a \vec{r}_{ao} = constant$

To eliminate the rotation of the molecule, its total angular momentum must be equated to zero.

$$\because \vec{M} = \sum m_a \vec{r}_a \times \vec{v}_a$$

$\because$ Velocity of a^{th} atom is $\vec{v}_a = \frac{d\vec{r}_a}{dt} = \frac{d(\vec{r}_{ao} + \vec{\varepsilon}_a)}{dt} = \dot{\vec{\varepsilon}}_a$

$$\therefore \vec{M} = \sum_a m_a \vec{r}_a \times \dot{\vec{\varepsilon}}_a = \sum_a m_a(\vec{r}_{ao} + \vec{\varepsilon}_a) \times \dot{\vec{\varepsilon}}_a$$

For small oscillations $\vec{M} \cong \sum_a m_a \vec{r}_{ao} \times \dot{\vec{\varepsilon}}_a$

$$\vec{M} = \frac{d}{dt} \sum_a m_a \vec{r}_{ao} \times \vec{\varepsilon}_a$$

The condition for $\vec{M}$ to be zero as : $\sum_a m_a \vec{r}_{ao} \times \vec{\varepsilon}_a = \text{constant}$

We can choose origin arbitrarily such that above constant becomes zero i.e.

$$\sum_a m_a \vec{r}_{ao} \times \vec{\varepsilon}_a = 0$$

If all n atoms lie in one plane i.e. for two dimensional case total degrees of freedom of n atoms is 2n . There will be two degrees of freedom of translational motion and one degree of freedom of rotational motion as angular velocity of system of n atoms will be only perpendicular to given plane. Then degrees of freedom of vibration = $2n - [2 \text{ (translation)} + 1 \text{ (rotational)}] = 2n - 3$. The number

of degrees of freedom $f_{2D\to 3D}^{vib}$ which correspond to vibrations in which atoms move out of the plane (i.e. motion becomes three dimensional from two dimensional) is

$$f_{2D\to 3D}^{vib} = f_{3D}^{vib} - f_{2D}^{vib} = (3n - 6) - (2n - 3) = n - 3.$$

For a linear molecule we distinguish longitudinal vibrations, which maintain the linear form, from vibrations which bring atoms out of the line.

Since a motion of n particles lie in a line corresponds to n degrees of freedom, of which one is translational, the number of vibrations which leave the atoms in a line in $n-1$.

Since the total number of vibrational degrees of freedom of a linear molecule is $3n-5$, there are $f_{1D\to 3D}^{vib}$ degrees of freedom which bring the atoms out of line. Thus $f_{1D\to 3D}^{vib} = f_{3D}^{vib} - f_{1D}^{vib} = (3n-5)-(n-1) = 2n-4$

There $2n-4$ vibration, however correspond to only $n-2$ different frequencies, since each vibrations can occur in two mutually perpendicular planes through the axis of the molecule.

5.7 Self Learning Exercise-II

Q.1 Find the ratio of frequencies ω and ω' of the oscillations of two diatomic molecules consisting of atoms of different isotopes, the masses of the atoms being m_1, m_2 and m_1', m_2'.

Q.2 The number of degrees of freedom of vibration of a molecule in which n atoms are collinear is

(A) $3n$ (B) $3n-6$ (C) $3n-5$ (D) $3n-4$

Q.3 Two masses m_1 and m_2 are connected by a spring of force constant k.The spring is compressed and released .Find the frequency of oscillation of the system.

5.8 Summary

We have considered small oscillations of a mechanical system about a position of stable equilibrium. We have also discussed oscillations of a system on which a variable external force acts. We have found that the energy transmitted to the system is determined by the squared modulus of the Fourier component of the force F (t) whose frequency is the intrinsic frequency of the system. We have also

carried out normal mode analysis of the oscillations of systems having more than one degree of freedom.

5.9 Glossary

Equilibrium: A state in which opposing forces or influences are balanced

Longitudinal :Running lengthwise rather than across:

5.10 Answers to Self Learning Exercises

Answers to Self Learning Exercise-I

Ans.1: $\omega = \sqrt{\frac{k}{m}}$ where $m = \frac{m_1 m_2}{m_1 + m_2}$

Ans.3: $\omega = \sqrt{\frac{k(m_1 + m_2)}{m_1 m_2}}$

Ans.4: $a = \sqrt{x_0^2 + \frac{v_0^2}{\omega^2}}$, $\tan\alpha = -\frac{v_0}{\omega x_0}$

Hint: Assume $x = a\cos(\omega t + \alpha)$, At $t = 0$ put $x = x_0$ *and* $\dot{x} = v_0$,

Answers to Self Learning Exercise-II

Ans.1: since the atoms of the isotopes interact in the same way, we have $k = k'$.

$\omega = \sqrt{\frac{k}{m}}$, where $m = \frac{m_1 m_2}{m_1 + m_2}$ and $\omega' = \sqrt{\frac{k}{m'}}$, where $m' = \frac{m_1' m_2'}{m_1' + m_2'}$

Hence $\frac{\omega'}{\omega} = \sqrt{\frac{m_1 m_2 (m_1' + m_2')}{m_1' m_2' (m_1 + m_2)}}$

Ans.2 : C

Ans.3: $\omega = \sqrt{\frac{k(m_1 + m_2)}{m_1 m_2}}$

5.11 Exercise

Q.1 The masses of the bobs of two pendulums are m_1 and m_2. The bobs are coupled by a spring of force constant k. If their lengths are equal to l,

the normal frequencies of the system are

(A) $\omega_1 = \sqrt{\frac{g}{l}}$; $\omega_2 = \sqrt{\frac{g}{l} + \frac{2k}{m}}$ (B) $\omega_1 = \sqrt{\frac{g}{l}}$; $\omega_2 = \sqrt{\frac{g}{l} + \frac{k}{m}}$

(C) $\omega_1 = \sqrt{\frac{g}{l}}$; $\omega_2 = \sqrt{\frac{g}{l}}$ (D) $\omega_1 = \sqrt{\frac{g}{2l}}$; $\omega_2 = \sqrt{\frac{k}{m}}$

Q.2 In planar molecule in which all *n* atoms lie in one plane, then degrees of freedom of vibration in which atoms lie in one plane are

(A) $2n$ (B) $2n-2$ (C) $2n-3$ (D) $2n-4$

Q.3 In above question the number of degrees of freedom which correspond to vibrations in which atoms move out of the plane are

(A) $2n$ (B) $n-3$ (C) n (D) $3n-6$

Q.4 A particle of the mass m moves in a constant vertical gravitational field along the path $y=ax^4$,where y is the vertical direction. Obtain the equation of motion for small oscillations about the position of the equilibrium.

Q.5 Find the normal coordinates of the system with following Lagrangian

(i) $L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}(\omega_1^2 x^2 + \omega_2^2 y^2) + \alpha xy$

(ii) $L = \frac{1}{2}(m_1\dot{x}^2 + m_2\dot{y}^2) - \frac{1}{2}(x^2 + y^2) + \beta\dot{x}\dot{y}$

Where $\alpha, \beta, \omega_1, \omega_2, m_1 \text{ and } m_2 \text{ are}$ constants.

5.12 Answers to Exercise

Ans.1: A Ans.2: C Ans.3: B

References and Suggested Readings

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UNIT-6
Motion of a Rigid Body

Structure of the Unit

6.0 Objectives

6.1 Introduction

6.2 Angular Velocity

6.3 The Inertia Tensor

6.4 Illustrative Examples

6.5 Self Learning Exercise-I

6.6 Angular Momentum of a Rigid Body

6.7 The Equations of Motion of a Rigid Body:

6.8 Self Learning Exercise-II

6.9 Summary

6.10 Glossary

6.11 Answers to Self Learning Exercises

6.12 Exercise

6.13 Answers to Exercise

6.14 References and Suggested Readings

6.0 Objectives

In this chapter we will consider any rigid body as a system of mass points subjected to the constraints that the distances between all pairs of points remain constant throughout the motion. We shall focus upon the following topics :

1. Relation between time rate of change of a vector in an inertial frame and the time rate of change of the same vector in a rotating frame.
2. The rigid body as a mechanical system with six degrees of freedom.
3. Independence of the angular velocity of rotation, at any instant, of a system of coordinates fixed in the body.

4. Angular velocity of the body.
5. Lagrangian of a rigid body.
6. Expression for kinetic energy of rotation.
7. Inertia tensor, principal axes of inertia.
8. Symmetrical, asymmetrical, spherical top, rotator.
9. Principal moments of inertia.
10. Angular momentum of a rigid body, precession of a Top.

6.1 Introduction

In case of the motion of a rigid body we can neglect the change in shape, size of the body. Any arbitrary motion of a rigid body can be treated as the composite of translation followed by rotation about some point O. The magnitude of translation can be arbitrary but rotation is absolute. We shall find an expression for inertia tensor and derive the general expression for the kinetic energy of rotation in terms of Eulerian angular velocity vector. We shall explain the precession of a top with the help of Euler's equations. We shall introduce pseudo forces which discussing the motion of a particle or body in non inertial frame e.g. accelerated and rotating frames.

6.2 Angular Velocity

A rigid body is defined as a system of particles such that the distance between the particles do not vary. To describe the motion of a rigid body, we use two systems of co-ordinates : a "fixed" (i.e. inertial) system XYZ, and a "moving system" $x_1 = x,\ x_2 = y,\ x_3 = z$ which is supposed to be rigidly fixed in the body and to participate in its motion(Fig.6.1). The origin of the moving system may be conveniently taken to be the centre of mass of the rigid body.

The position of the rigid body with respect to the fixed system of coordinates is completely determined if the position of the moving system is specified.

Let the origin O of the moving system have the radius vector $\vec{R}$ with respect to fixed system (figure 6.1)

The orientation of the axes x_1, x_2, x_3 of the moving system relative to the fixed system is given by three independent angles, which together with the three

components of the vector $\vec{R}$ make six co-ordinates. Thus a rigid body is a mechanical system with six degrees of freedom.

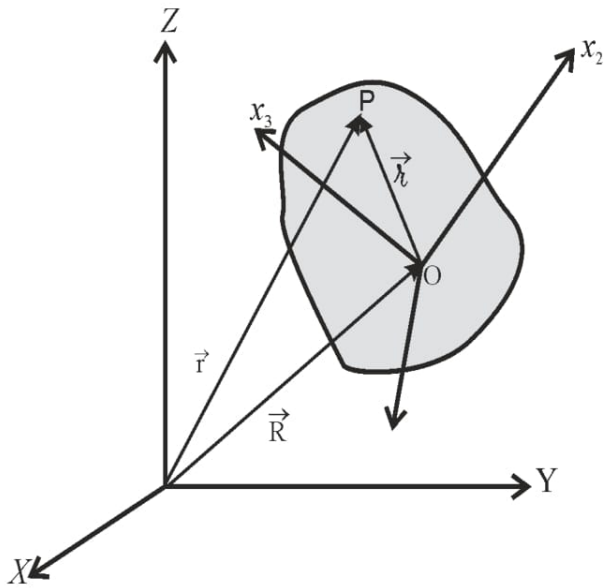


Figure 6.1 *XYZ* is fixed inertial system and $x_1x_2x_3$ moving system rigidly fixed in the rigid body

Let us consider an arbitrary infinitesimal displacement of a rigid body. It can be represented as the sum of two parts, one of these is an infinitesimal translation of the rigid body, whereby the centre of mass moves to its final position, but the orientation of the axes of the moving system of coordinates is unchanged. The other is an infinitesimal rotation about the centre of mass(i.e. orientation of axes of the moving system $x_1x_2x_3$ changes),but coordinates of the centre of mass remains unchanged .

Let $\vec{\lambda}$ be the radius vector of an arbitrary point in a rigid body with respect to origin of the moving system, and $\vec{r}$ the radius vector of the same point with respect to origin of the fixed system XYZ. With respect to fixed system XYZ, infinitesimal displacement of the point P is $d\vec{r}$ which consists of displacement, $d\vec{R}$ equal to that of the centre of mass, and a displacement $d\vec{\phi} \times \vec{\lambda}$ relative to the centre of mass resulting from rotation through an infinitesimal angle $d\vec{\phi}$:

$$d\vec{r} = d\vec{R} + d\vec{\phi} \times \vec{\lambda} \qquad (6.1)$$

Displacement of the point P with respect to fixed XYZ system =

{(Displacement of the origin of the moving system with respect to fixed XYZ system)+(Displacement of the point P with respect to the origin of the moving system)}

$$\frac{d\vec{r}}{dt} = \frac{d\vec{R}}{dt} + \frac{d\vec{\phi}}{dt} \times \vec{\imath}$$

$$\boxed{\vec{v} = \vec{V} + \vec{\Omega} \times \vec{\imath}} \qquad (6.2)$$

Where

$$\frac{d\vec{r}}{dt} = \vec{v}, \frac{d\vec{R}}{dt} = \vec{V}, \qquad \frac{d\vec{\phi}}{dt} = \vec{\Omega}$$

$\vec{v}$= Velocity of the point P of the rigid body with respect to fixed XYZ system

$\vec{V}$ =Velocity of the origin *O* (of the moving system $x_1x_2x_3$) with respect to fixed XYZ system

If we consider origin *O* as the centre of mass of the rigid body, then it is known as the‘ translational velocity’ of the rigid body.

The vector $\vec{\Omega}$ is called the “angular velocity” of the rotation of the body; its direction, like that of $d\vec{\phi}$, is along the axis of rotation. The point P of the rigid body is in pure rotation about origin *O* of the moving system.

$\vec{\Omega} \times \vec{\imath}$ is the velocity of the point P with respect to origin *O* of the moving system

By equation (6.2) we can say that the velocity $\vec{v}$ of any point in the body relative to the fixed system XYZ can be expressed in terms of the translational velocity of the rigid body and its angular velocity of rotation.

It should be emphasized that, in deriving formula (6.2), no use has been made of the fact that the origin is located at the centre of mass.

If we consider that the moving system of coordinates fixed in the body is such that its origin is not at the centre of mass O , but at some point of O' at a distance $\vec{a}$ from O. Let the velocity of O' be $\vec{V}'$ and the angular velocity of the new system of coordinates be $\vec{\Omega}'$.

We know that the angular velocity of rotation, at any instant, of a system of coordinates fixed in the body is independent of the particular system chosen i.e.

angular velocity of rigid body is same with respect to points O and O' because both points are rigidly attached to rigid body .Thus $\vec{\Omega}' = \vec{\Omega}$

We again consider the same point P in the body and denote $\vec{\imath}'$ by its position vector with respect of O'.

Thus $\vec{\imath} = \vec{\imath}' + \vec{a}$

Substituting in Eq. (6.2), we get

$$\vec{v} = \vec{V} + \vec{\Omega} \times (\vec{\imath}' + \vec{a})$$

$$= \vec{V} + \vec{\Omega} \times \vec{\imath}' + \vec{\Omega} \times \vec{a}$$

$$= (\vec{V} + \vec{\Omega} \times \vec{a}) + \vec{\Omega} \times \vec{\imath}'$$

$$\vec{v} = \vec{V}' + \vec{\Omega} \times \vec{\imath}' \quad \because \vec{\Omega} = \vec{\Omega}'$$

$$\vec{v} = \vec{V}' + \vec{\Omega}' \times \vec{\imath}' \tag{6.3a}$$

Where $\vec{V}' = \vec{V} + \vec{\Omega} \times \vec{a}$, (6.3b)

Here $\vec{V}$= velocity of the CM of the rigid body with respect to fixed system

$\vec{\Omega} \times \vec{a}$ = velocity of O' with respect to CM of the rigid body .

$\vec{V}' = \vec{V} + \vec{\Omega} \times \vec{a}$ = Velocity of O' with respect to fixed system XYZ

$\vec{\Omega}' \times \vec{\imath}'$ = Velocity of the point P with respect to O'

We can choose $\vec{a}$ such that the term $\vec{V} + \vec{\Omega} \times \vec{a}$ becomes zero, Thus it is then always possible to choose an origin O' whose velocity $\vec{V}'$ is zero, then from equation (6.3a) $\vec{v} = \vec{\Omega}' \times \vec{\imath}'$ .So the motion of the body at the instant considered is a pure rotation about an axis through O'(because at that instant of time O' is at rest).This is called the instantaneous axis of rotation.

6.3 The Inertia Tensor

The kinetic energy T of a rigid body with respect to fixed XYZ System can be expressed as

i.e. $T = \sum \frac{1}{2} mv^2$, where sum is over all the particles comprising the body.

Here we assume that centre of mass of the rigid body be origin of the moving system .

From eq.(6.2)

$$\vec{v} = \vec{V} + \vec{\Omega} \times \vec{r}$$

$$T = \sum \frac{1}{2} mv^2 = \sum \frac{1}{2} m [\vec{V} + \vec{\Omega} \times \vec{r}]^2$$

$$T = \sum \frac{1}{2} mV^2 + \sum m \vec{V}.\left(\vec{\Omega} \times \vec{r}\right) + \frac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

$$= \tfrac{1}{2} V^2 \sum m + \sum m \vec{V}.\left(\vec{\Omega} \times \vec{r}\right) + \tfrac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

where $\sum m = \mu$

$$T = \tfrac{1}{2} \mu V^2 + \sum m \vec{V}.\left(\vec{\Omega} \times \vec{r}\right) + \tfrac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2 \qquad (6.4)$$

By scalar product $\vec{V}.(\vec{\Omega} \times \vec{r}) = \left[\vec{V}\,\vec{\Omega}\,\vec{r}\right] = \left[\vec{\Omega}\,\vec{r}\,\vec{V}\right] = \vec{\Omega}.\left(\vec{r} \times \vec{V}\right)$

Putting this value in eq.(6.4)

$$T = \frac{1}{2} \mu V^2 + \sum m \vec{\Omega}.\left(\vec{r} \times \vec{V}\right) + \frac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

$$T = \frac{1}{2} \mu V^2 + \vec{\Omega}.\sum \left(m \vec{r} \times \vec{V}\right) + \frac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

(Since $\vec{\Omega}$ is same for all the particles of the rigid body)

$$T = \frac{1}{2} \mu V^2 + \vec{\Omega}.\sum m \vec{r} \left(\times \vec{V}\right) + \frac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

$$T = \tfrac{1}{2} \mu V^2 + \vec{\Omega}.[(\sum m \vec{r}) \times \vec{V}] + \tfrac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2$$

Since CM is at origin so $\vec{r}_{CM} = \dfrac{\sum m \vec{r}}{\sum m} = \vec{0}$ *i.e.* $\sum m \vec{r} = \vec{0}$

$$\boxed{T = \frac{1}{2} \mu V^2 + \frac{1}{2} \sum m (\vec{\Omega} \times \vec{r})^2} \qquad (6.5)$$

$$\boxed{T = \frac{1}{2} \mu V^2 + \frac{1}{2} \sum m v_{rel\ to\ CM}^2}$$

Here $\vec{v}_{rel\ toCM} = \vec{\Omega} \times \vec{r}$

T=K.E. of Translational motion + K.E. of rotational motion with angular velocity Ω about on axis passing through the centre of mass.

It should be emphasized that this division of the K.E. into two parts is possible only because the origin of the coordinate system fixed in the body has been taken to be at the CM. We can write total kinetic energy as

$$\boxed{T = KE_{ofCM} + KE_{About\ CM}}$$

We can write

$$\left(\vec{\Omega} \times \vec{\imath}\right)^2 = \left(\Omega \imath \sin\theta\right)^2 = \Omega^2 \imath^2 \sin^2\theta = \Omega^2 \imath^2 (1 - \cos^2\theta)$$

$$= \Omega^2 \imath^2 - \Omega^2 \imath^2 \cos^2\theta = \Omega^2 \imath^2 - \left(\vec{\Omega}.\vec{\imath}\right)^2$$

Putting this value in eq.(6.5)

$$T = \frac{1}{2}\mu V^2 + \frac{1}{2}\sum m \left[\Omega^2 \vec{\imath}^{\,2} - (\vec{\Omega}.\vec{\imath})^2\right]$$

We may rewrite the Rotational K.E in tensor form i.e. in terms of the components x_i and Ω_i of the vector $\vec{\imath}$ and $\vec{\Omega}$.

$$T_{rot.} = \frac{1}{2}\sum m\ (\Omega_i^2 x_i^2 - \Omega_i x_i \Omega_k x_k)$$

[Here $\Omega_i = \delta_{ik}\,\Omega_k$, (6.6)

where δ_{ik} is unit tensor whose components are unity for i =k and zero for i≠ k]

$$T_{rot.} = \frac{1}{2}\sum m\ [\Omega_i(\Omega_k \delta_{ik}) x_l^2 - \Omega_i \Omega_k x_i x_k]$$

$$= \frac{1}{2}\Omega_i \Omega_k \sum m\left(x_l^2\ \delta_{ik} - x_i x_k\right)$$

$$T_{rot.} = \tfrac{1}{2}\Omega_i \Omega_k I_{ik} \quad (6.7)$$

where $I_{ik} = \sum m\left(x_l^2\ \delta_{ik} - x_i x_k\right)$ (6.8)

(Note i, k, l are tensor suffixes and take values 1, 2, 3.

Here $A_i B_i = \vec{A}.\vec{B},\ A_l^2 = \vec{A}^2$)

Thus total kinetic energy $T = T_{trans} + T_{rot}$

$$\boxed{T = \frac{1}{2}\mu V^2 + \frac{1}{2} I_{ik}\Omega_i \Omega_k}$$

Lagrangian of the system $L = T - U$

$$L = \frac{1}{2}\,\mu V^2 + \frac{1}{2} I_{ik}\,\Omega_i \Omega_k - U$$

The P.E. is in general a function of the six variables which define the position of the rigid body e.g. the three coordinates X, Y, Z of C.M. and three angles which specify the relative orientation of the moving and fixed coordinate axes.

Here inertia tensor of rigid body $\boxed{I_{ik} = \sum m\left(x_l^2 \delta_{ik} - x_i x_k\right)}$

It is symmetrical ,thus $\boxed{I_{ik} = I_{ki}}$

It is evident from above expression of I_{ik}

$$\boxed{I_{ik} = \begin{bmatrix} \sum m\left(y^2 + z^2\right) & -\sum m\, xy & -\sum m\, xz \\ -\sum m\, yx & \sum m\left(x^2 + z^2\right) & -\sum m\, yz \\ -\sum m\, zx & -\sum m\, zy & \sum m\left(x^2 + y^2\right) \end{bmatrix}}$$

I_{xx} , I_{yy} , I_{zz} are called moment of Inertia about the corresponding axis. If the body is regarded as continuous, the sum in the definition I_{ik} becomes in integrals over the volume of the body .

$$\boldsymbol{I_{ik} = \int \rho \left(x_l^2 \delta_{ik} - x_i x_k\right) dV}$$

Here dV is volume elememt and ρ is the mass density.

From eq.(6.7)

$$T_{rot.} = \frac{1}{2}\Omega_i \Omega_k I_{ik}$$

$$T_{rot.} = \tfrac{1}{2}\left[I_{xx}\,\Omega_x\Omega_x + I_{xy}\,\Omega_x\Omega_y + I_{xz}\,\Omega_x\Omega_z + I_{yy}\,\Omega_y\Omega_y + I_{yx}\,\Omega_y\Omega_x + I_{yz}\,\Omega_y\Omega_z + I_{zx}\,\Omega_z\Omega_x + I_{zy}\,\Omega_z\Omega_y + I_{zz}\,\Omega_z\Omega_z\right] \quad (6.8)$$

Here $\boxed{I_{yx} = I_{xy}, I_{xz} = I_{zx}, I_{yz} = I_{zy}}$

$$\therefore\ T_{rot.} = \frac{1}{2}\left[I_{xx}\,\Omega_x^2 + I_{yy}\Omega_y^2 + I_{zz}\Omega_z^2 + 2I_{xy}\,\Omega_x\Omega_y + 2I_{yz}\,\Omega_y\Omega_z + 2I_{zx}\,\Omega_z\Omega_x\right]$$

$$\therefore\ T_{rot.} = \frac{1}{2}\left[I_{11}\,\Omega_1^2 + I_{22}\Omega_2^2 + I_{33}\Omega_3^2 + 2I_{13}\,\Omega_1\Omega_3 + 2I_{23}\,\Omega_2\Omega_3 + 2I_{31}\,\Omega_3\Omega_1\right]$$

Like any ***symmetrical tensor of ranks two***, the inertia tensor can be reduced to diagonal form by an appropriate choice of the directions of the axis x_1, x_2, x_3. ***These directions are called Principal axes of inertia and the corresponding values of the diagonal components are principal moment of inertia***. We denote them by I_1, I_2, I_3 when the axes x_1, x_2, x_3 are so chosen .In that case

$$I_{xx} = I_{11} = I_1 \quad , \; I_{yy} = I_{22} = I_2 \quad , \quad I_{zz} = I_{33} = I_3$$

$$I_{xy} = I_{xz} = I_{yz} = 0$$

For this case, in general $I_{ik} \neq 0 \; if \; i = k \;\; and \;\; I_{ik} = 0 \;\; if \;\; i \neq k$

Thus eq.(6.8) becomes $T_{Rot.} = \frac{1}{2}\left(I_1\Omega_1^2 + I_2\Omega_2^2 + I_3\Omega_3^2\right)$

None of the three principal moments of inertia can exceed the sum of the other two inertia. For instance

$$I_1 + I_2 = \sum m\,(x_2^2 + x_3^2) + \sum m\,(x_1^2 + x_3^2)$$

$$= \sum m\,(x_1^2 + x_2^2 + 2x_3^2) \geq \sum m(x_1^2 + x_2^2) = I_3$$

$\boldsymbol{I_1 \neq I_2 \neq I_3}$ ***asymmetrical top*** ,

$\boldsymbol{I_1 = I_2 = I_3}$ ***Spherical top***

$\boldsymbol{I_1 = I_2 \neq I_3}$ ***Symmetrical top***

The determination of the principal axes of inertia is much simplified if the body is symmetrical, for it is clear that position of the centre of mass and the directions of the principal axes must have the same symmetry as the body.

For example, if the body has a plane of symmetry, the centre of mass must lie in that plane which also contains two of the principal axes of inertia, while the third is perpendicular to the plane. An obvious case of this kind is a coplanar system of particles.

Here there is a simple relation between the three principal moments of inertia. If the plane of the system is taken as x_1, x_2 plane then $x_3 = 0$ for every particle and so $I_1 = \sum m x_2^2, I_2 = \sum m\, x_1^2, I_3 = \sum m\,(x_1^2 + x_2^2)$

$$\therefore \; I_3 = I_1 + I_2$$

If the body has an axis of symmetry of any order, the centre of mass must lie

on that axis, which is also one of the principal axes of inertia, while the other two are perpendicular to it. If the axis is of order higher than the second, the body is a

symmetrical top. For any principal axis perpendicular to the axis of symmetry can be turned through an angle different from 180° about the latter, i.e. the choice of the perpendicular axes is not unique, and this can happen only if the body is a symmetrical top.

A particular case here is a collinear system of particles. If the line of the system is taken as the x_3-axis then $x_1 = x_1 = 0$ for every particle and so $I_1 = I_2 = \sum m x_3^2$, $I_3 = 0$ such a system is called a rotator.

The characteristic property which distinguishes a rotator from other bodies is that it has only two, not three, rotational degrees of freedom, corresponding to rotations about the $x_1$and x_2-axes It is clearly meaningless to speak of the rotation of a straight line about itself, because moment of inertia of the body is about that straight line is zero.

Finally we may note the further result concerning the calculation of the inertia tensor.

Choose some other origin O':

$$I'_{ik} = \sum m\left(x_l'^2\ \delta_{ik} - x'_i x'_k\right)$$

From previous diagram $\because \overrightarrow{OO'} = \vec{a}$

$$\therefore\ \vec{\imath} = \vec{\imath}' + \vec{a}$$

$$x_1 = x_1' + a_1\,,$$

$$x_2 = x_2' + a_2\,,$$

$$x_3 = x_3' + a_3 \quad \text{i.e. } x_i = x_i' + a_i$$

or $x_i' = x_i - a_i\,, \quad and \sum m\vec{\imath} = 0 \quad (\because O\ is\ C.M.)$ i.e $\sum m\, x_i = 0$

$$I'_{ik} = \sum m\left(x_l'^2\ \delta_{ik} - x'_i x'_k\right)$$

$$I'_{ik} = \sum m[(x_l - a_l)^2\delta_{ik} - (x_i - a_i)(x_k - a_k)]$$

$$\therefore\ I'_{ik} = \sum m\,[(x_l^2 + a_l^2 - 2x_l a_i)\delta_{ik} - (x_i - a_i)(x_k - a_k)]$$

$$I'_{ik} = \sum m\,[(x_l^2\delta_{ik} + a_l^2\delta_{ik} - 2x_l a_i\delta_{ik}) - x_i x_k + x_i a_k + a_i x_k - a_i a_k]$$

$$I'_{ik} = \sum [m\,(x_l^2\delta_{ik} - x_i x_k)] + \sum [m\,(a^2\delta_{ik} - a_i a_k)] + \sum m\, x_i a_k + \sum m a_i x_k - \sum 2m x_l a_l \delta_{ik}$$

$$I'_{ik} = \sum [m\,(x_l^2\delta_{ik} - x_i x_k)] + (a^2\delta_{ik} - a_i a_k)\sum(m) + a_k \sum m\,x_i + a_i \sum m x_k - 2a_l\delta_{ik}\sum m x_l$$

Using $\sum m\,x_i = 0$ We get

$$I'_{ik} = \sum[m\,(x_l^2\delta_{ik} - x_i x_k)\,] + (a^2\delta_{ik} - a_i a_k)\sum(m) + a_k.0 + a_i.0 - 2a_l\delta_{ik}.0$$

$$I'_{ik} = \sum[m\,(x_l^2\delta_{ik} - x_i x_k)\,] + \mu(a^2\delta_{ik} - a_i a_k) \text{ where } \sum(m) = \mu$$

$$= I_{ik} + \mu[a^2\delta_{ik} - a_i a_k]$$

6.4 Illustrative Examples

Example 6.1 Find the principal moments of inertia of a hollow sphere about diameter.

Sol. By definition inertia tensor is

$$I_{ik} = \sum m(\mathrm{x}_l^2\,\delta_{ik} - \mathrm{x}_i\mathrm{x}_k)$$

As hollow sphere is three dimensionally symmetric body, so

$$I_1 = I_2 = I_3$$

Adding the diagonal terms

$$I_1 + I_2 + I_3 = 3I = \sum 2m(\mathrm{y}^2 + \mathrm{z}^2 + \mathrm{x}^2)$$
$$= \sum 2mR^2$$
$$= 2R^2M$$

Therefore $I = \frac{2}{3}MR^2$ Where M is the mass of hollows sphere.

Example 6.2 Find the principal moments of inertia of a homogenous solid sphere of radius R.

Sol. $I_1 = I_2 = I_3$; Therefore calculating the sum

$I_1 + I_2 + I_3 = 2\rho\int r^2.dV$, ρ is density

$$3I = 2\frac{M}{\frac{4}{3}\pi R^3}\int_0^R r^2.4\pi r^2 dr$$

$$3I = \frac{2M}{\frac{4}{3}\pi R^2} 4\pi \frac{R^5}{5}$$

$$I = \frac{2}{5} MR^2$$

Example 6.3 Determine the principal moments of inertia for the following types of molecules regarded as systems of particles at fixed distances apart :

(a) a molecule of collinear atoms

(b) a triatomic molecule which is an isosceles triangle.

(c) a tetra atomic molecule which is an equilateral based tetrahedron.

Sol.(a) $I_1 = I_2 = \frac{1}{M} \sum_{a \neq b} m_a m_b l_{ab}^2, \quad I_3 = 0$

Where m_a is the mass of the ath and bth atoms, and the summation includes one term for every pair of atoms in the molecule.

For diatomic molecule there is only one term in the sum and the result is

$$I_1 = I_2 = \frac{m_1 m_2}{m_1 + m_2} l^2$$

(b) The centre of mass is on the axis of symmetry of the triangle, at a distance $X_2 = \frac{m_2 h}{\mu}$ from its base (h being the height of the triangle and μ is the total mass of the molecule $2m_1 + m_2$)

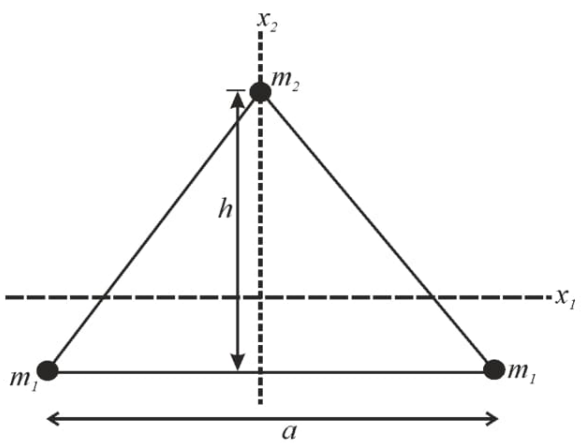


Figure 6.2

The moments of inertia are $I_1 = \frac{2m_1m_2h^2}{\mu}, I_2 = \frac{1}{2}m_1a^2, I_3 = I_1 + I_2$

(c) The centre of mass is on the axis of symmetry of the tetrahedron at a distance $X_3 = \frac{m_2h}{\mu}$ from its base (*h* being the height of the tetrahedron)

$$I_1 = I_2 = \frac{3m_1m_2h^2}{\mu} + \frac{1}{2}m_1a^2, I_3 = m_1a^2.$$

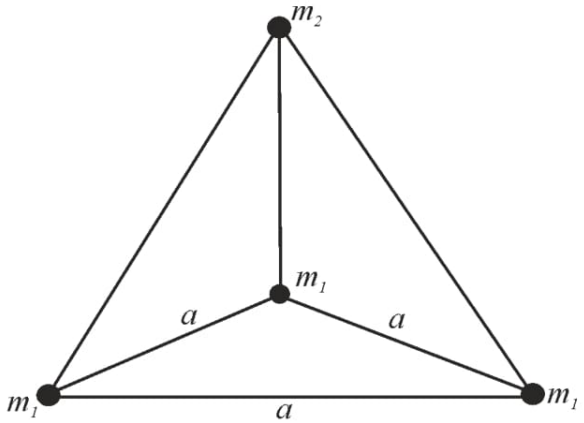


Figure 6.3

If $m_1 = m_2, h = \sqrt{\frac{2}{3}}a$, then molecule is a regular tetrahedron and

$I_1 = I_2 = I_3 = m_1a^2$.

6.5 Self Learning Exercise -I

Section A :Very Short Answer Type Questions

Q.1 Determine the principal moments of inertia for a thin rod of length *l*.

Q.2 Define Inertia tensor. Write expressions for I_{11}, I_{22}, I_{33}.

Q.3 State theorems of parallel and perpendicular axes.

Q.4 Write expression for kinetic energy of a rigid body.

Section B: Short Answer Type Questions

Q.5 Define inertia tensor. Derive an expression for kinetic energy of rotation as

$$T_{rot} = \frac{1}{2}\Omega_i\Omega_k I_{ik}$$

Q.6 Determine the principal moments of inertia of a circular cylinder of radius R and height *h*.

6.6 Angular Momentum of a Rigid Body and Precessional Motion

Choose origin of the moving coordinate system at CM of the rigid body about which we have to calculate the Angular momentum about centre of mass

$$\vec{M} = \sum m\vec{\imath} \times \vec{v}_{rel\ to\ CM}$$

$$= \sum m\vec{\imath} \times (\vec{\Omega} \times \vec{\imath})$$

$$= \sum m[\vec{\imath}^{\,2}\ \vec{\Omega} - \vec{\imath}(\vec{\imath}\,.\vec{\Omega}) \qquad \because \vec{A}\times(\vec{B}\times\vec{C}) = \vec{B}(\vec{A}.\vec{C}) - \vec{C}(\vec{A}.\vec{B})$$

$$\vec{M} = \sum m[(x_1^2 + x_2^2 + x_3^2)(\Omega_1\hat{i} + \Omega_2\hat{j} + \Omega_1\hat{k})$$
$$-(x_1\hat{i} + x_2\hat{j} + x_3\hat{k})(x_1\Omega_1 + x_2\Omega_2 + x_3\Omega_3)]$$

ith component $M_i = \sum m[(x_1^2 + x_2^2 + x_3^2)\Omega_1 - x_1(x_1\Omega_1 + x_2\Omega_2 + x_3\Omega_3)]$

In tensor notation

$$M_i = \sum m\,[x_l^2\Omega_i - x_i(x_k\Omega_k)]$$

$$M_i = \sum m\,[x_l^2\Omega_i - x_i x_k\Omega_k]$$

$$M_i = \sum m\,[x_l^2\Omega_k\delta_{ik} - x_i x_k\Omega_k] \qquad \because \text{From (6)} \quad \Omega_i = \delta_{ik}\,\Omega_k$$

$$= \Omega_k \sum m\,(x_l^2\delta_{ik} - x_i x_k) \quad \text{By eq.(6.8)we have}$$

$$M_i = I_{ik}\,\Omega_k$$

Thus $M_1 = I_{11}\,\Omega_1 + I_{12}\,\Omega_2 + I_{13}\,\Omega_3$

$M_2 = I_{21}\,\Omega_1 + I_{22}\,\Omega_2 + I_{23}\,\Omega_3$

$M_3 = I_{31}\,\Omega_1 + I_{32}\,\Omega_2 + I_{33}\,\Omega_3$

If $x_1x_2x_3$ are the same as the principal axes of inertia,

then $I_{12} = I_{13} = I_{23} = 0,\ \ I_{11} = I_1\ ,\ I_{22} = I_2\ ,I_{33} = I_3$

So $M_1 = I_1\,\Omega_1\ ,M_2 = I_2\,\Omega_2\ ,\ M_3 = I_3\,\Omega_3$

In particular for a spherical top $I_1 = I_2 = I_3 = I$

$$M_1 = I\Omega_1\ ,M_2 = I\Omega_2\ ,\qquad M_3 = I\Omega_3$$

$$\vec{M} = M_1\hat{i} + M_2\hat{j} + M_3\hat{k} = I\,\Omega_1\hat{i} + I\,\Omega_2\hat{j} + I\,\Omega_3\hat{k}$$
$$= I\left(\Omega_1\hat{i} + \Omega_2\hat{j} + \Omega_3\hat{k}\right) = I\,\vec{\Omega}$$

Here $\vec{M}$ and $\vec{\Omega}$ are in same direction and proportional.

$\vec{M}$ is not in general in the same direction as $\vec{\Omega}$,this happens only when the body is rotating about one of its principal axes of inertia.

Let us consider a rigid body moving freely, i.e. not subject to any external forces. We suppose that any uniform translational motion, which is of no interest, is removed, leaving a free rotation of the body.

As in any closed system, the angular momentum of the freely rotating body is constant. For a spherical top the condition $\vec{M}$ = constant gives $\vec{\Omega}$ = constant i.e. the most general free rotation of a spherical top is a uniform rotation about an axis fixed in space.

The case of rotator is equally simple. Here also $\vec{M} = I\vec{\Omega}$ and the vector$\vec{\Omega}$ is perpendicular to the axis of the rotator. Hence a free rotation of a rotator is a

uniform rotation in one plane about an axis perpendicular to the plane.

The law of conservation of angular momentum also suffices to determine the more complex free rotation of a symmetrical top. Using the fact that the principal axes of inertia x_1, x_2 (perpendicular to the axis of symmetry of (x_3) of the top) may be chosen arbitrarily, we take the x_2-axis perpendicular to the plane containing the constant $\vec{M}$ vector and the instantaneous position of the x_3-axis.

Then $M_2 = 0$ $\quad\therefore$ Using $M_2 = I_2\Omega_2$ *we get* $\Omega_2 = 0$

This means that the directions of $\vec{M}$, $\vec{\Omega}$ and the axis of the top are at every instant in one plane.

Hence, in turn, it follows that the velocity $\vec{v}_{rel\ to\ CM} = \vec{\Omega} \times \vec{r}$ of every point on the axis of the top is at every instant perpendicular to that plane.

That is, the axis of the top rotates uniformly about the direction of $\vec{M}$,describing a circular cone. This is called regular precession of the top.

At the same time the top rotates uniforms about its own axis.

The angular velocities of these two rotations can easily be expressed in terms of the given angular momentum $\vec{M}$ and the angle θ between the axis of the top and direction of $\vec{M}$ vector.

The angular velocity of the top about its own axis is just the component Ω_3 of the vector $\vec{\Omega}$ along the axis.

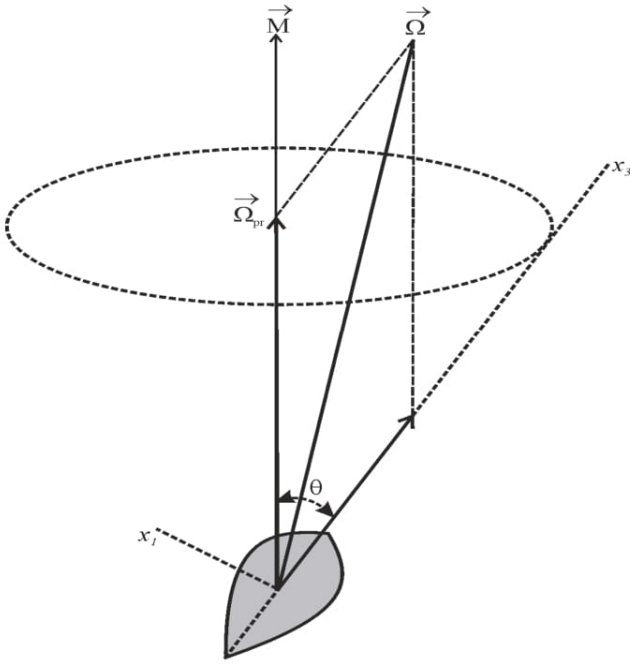


Figure 6.4

$\because \Omega_3 = \frac{M_3}{I_3} = \frac{M}{I_3}.\cos\theta$.To determine the rate of precession Ω_{pr}, the vector $\vec{\Omega}$ must be revolved into components along x_3 and along $\vec{M}$. The first of these gives no displacement of the axis of the top, and the second component is therefore the required angular velocity of precession.

Note that $\Omega_{pr}\sin\theta = \Omega_1 = \frac{M_1}{I_1}$

$$= \frac{M\sin\theta}{I_1}$$

Thus $\Omega_{pr} = \frac{M}{I_1}$

6.7 The Equations of Motion of a Rigid Body

Since ***rigid body has in general, six degrees of freedom***, the general equations of motion must be six in number.

They can be put in form which gives the time derivative of two vectors, the momentum and angular momentum of the body.

The first equation is simply summing the equations $\dot{\vec{p}} = \vec{f}$ for each particle in the body. Here $\vec{f}$ is the force acting on the particle and $\dot{\vec{p}}$ is the rate of change of the momentum of the particle.

Total momentum of the rigid body =(total mass of the body) velocity of CM of the body i.e.

$\vec{P} = \sum \vec{p} = \mu \vec{V}$ The total force $= \sum \vec{f} = \vec{F}$ or $\frac{d\vec{P}}{dt} = \vec{F}$

$\vec{F}$ has been defined as the sum of all forces $\vec{f}$ acting on the various particles, including the forces due to other particles, $\vec{F}$ actually includes only external forces : the forces of interaction(internal forces) between the other particles composing the body cancel out.

If U is the P.E. of the rigid body in an external field, then force acting on the rigid body is $\vec{F} = -\frac{\partial U}{\partial \vec{R}}$

Here U is differentiated with respect to coordinates of center of mass of the body.

∵ When the body undergoes translation through a distance $\delta\vec{R}$ the radius vector $\vec{r}$ of every point in the body changes by $\delta\vec{R}$ so that change in the P.E. is

$$\delta U = \sum \left(\frac{\partial U}{\partial \vec{r}}\right) . \delta\vec{r} = \delta\vec{R} . \sum \frac{\partial U}{\partial \vec{r}} = -\delta\vec{R} . \sum \vec{f} = -\vec{F} . \delta\vec{R}$$

Here $\vec{r} = \vec{R} + \vec{\kappa}$ $or\ \delta\vec{r} = \delta\vec{R} + 0 = \delta\vec{R}$

For translation $\delta\vec{\kappa} = 0$ i.e. displacement of particle with respect to CM of the body is zero in translatory motion .

$$\delta U = \sum \left(\frac{\partial U}{\partial \vec{r}}\right) . \delta\vec{r} = \sum \left(\frac{\partial U}{\partial \vec{r}}\right) . \delta\vec{R} = \delta\vec{R} . \sum \left(\frac{\partial U}{\partial \vec{r}}\right)$$
$$= \delta\vec{R} . \left[\sum -\vec{f}\right] = -\left[\sum \vec{f}\right] . \delta\vec{R} = -\vec{F} . \delta\vec{R}$$

6.8 Self Learning Exercise-II

Section A : Very Short Answer Type Questions

Q.1 Write the Lagrangian for a rigid body.

Q.2 What is a spherical Top?

Q.3 Are angular momentum vector $\vec{M}$ and angular velocity vector $\vec{\Omega}$ co-directional?

Section B : Short Answer Type Questions

Q.4 Justify that angular momentum $\vec{M}$ is not in general in the same direction as $\vec{\Omega}$.

Q.5 Prove the relation.

$$d\vec{r} = d\vec{R} + d\vec{\phi} \times \vec{r}$$

Q.6 Explain the regular precession of a symmetric top.

6.9 Summary

In this chapter we have discussed the following :

(a) A rigid body is a dynamical system having six degrees of freedom : three correspond to translation and three correspond to rotation.

(b) Velocity of a particle attached to the body in motion is given by

$$\vec{v} = \vec{V} + \vec{\Omega} \times \vec{r}$$

(c) $$K.E. = \frac{1}{2}\mu V^2 + \frac{1}{2}\sum m[\Omega^2 \mathrm{r}^2 - (\vec{\Omega}.\vec{r})^2]$$

$$= \frac{1}{2}\mu V^2 + \frac{1}{2} I_{ik} \Omega_i \Omega_k$$

(d) The Lagrangian for a rigid body is

$$L = \frac{1}{2}\mu V^2 + \frac{1}{2} I_{ik} \Omega_i \Omega_k - U$$

(e) Angular momentum of a rigid body is $M_i = I_{ik}\Omega_k$

6.10 Glossary

Arbitrary **:** (Of a constant or other quantity) of unspecified value.

Collinear **:** (Of points) lying in the same straight line.

Infinitesimal **:** An indefinitely small quantity; a value approaching zero.

Precession **:** The slow movement of the axis of a spinning body around another axis due to a torque (such as gravitational influence) acting to change the direction

of the first axis .

Translation **:** Movement of a body from one point of space to another such that every point of the body moves in the same direction and over the same distance, without any rotation, reflection, or change in size.

6.11 Answer to Self Learning Exercises

Answer to Self Learning Exercise-I

Ans.1: $I_1 = I_2 = \frac{1}{12}Ml^2, I_3 = 0$ (We neglect the thickness rod)

Ans.3: Theorem of perpendicular axes : $I_3 = I_1 + I_2$

Theorem of parallel axes : $I = I_{cg} + Ma^2$

Ans.6: $I_1 = I_2 = \frac{M}{4}(\mathrm{R}^2 + \frac{h^2}{3}), \mathrm{I}_3 = \frac{1}{2}MR^2$ (Where $x_3 -$axis is along the axis of the cylinder).

Answer to Self Learning Exercise-II

Ans.2: $I_1 = I_2 = I_3$ (Spherical Top)

Ans.3 (No in general)

6.12 Exercise

Section A : Very Short Answer Type Questions

Q.1 What is a symmetrical, asymmetrical, spherical Top?

Q.2 Is moment of inertia tensor Symmetric?

Q.3 What is a rotator?

Section B : Short Answer Type Questions

Q.4 Determine the moments of inertia of a diatomic molecule.

Q.5 Derive K.E. of rotation of a rigid body: $T = \frac{1}{2}I_{ik}\Omega_i\Omega_k$

Section C : Long Answer Type Questions

Q.6 (a) Derive an expression for kinetic energy of a rigid body in terms of inertia tensor. Show that inertia tensor is symmetric $(\mathrm{I}_{ik} = \mathrm{I}_{ki})$.

(b) Determine the principal moments of inertia of a triatomic molecule which is an isosceles triangle.

Q.7 (a) Derive an expression for the angular momentum of a rigid body in terms of inertia tensor.

(b) Discuss the free rotation of a symmetrical top. Show that the angular velocity of precession is given by $\Omega_{precession} = \frac{M}{I_1}$

Q8. (a) Derive the equations of motion of a rigid body :

$$\frac{d\vec{P}}{dt} = \vec{F} \text{ and } \frac{d\vec{M}}{dt} = \vec{K}$$

(b) Also show that the above equations of motion of a rigid body can also be obtained by the Lagrange's equation where the Lagrangian of the rigid body is

$$L = \frac{1}{2}\mu V^2 + \frac{1}{2} I_{ik}\Omega_i \Omega_k - U$$

6.13 Answers to Exercise

Ans.3 Yes $(I_1 = I_2, I_3 = 0)$

6.14 References and Suggested Readings

1. L.D. Landau and E. M. Lifshitz, Mechanics, Butterworth- Heinemann

2. Gupta ,Kumar &Sharma ,Classical Mechanics, Pragati Prakashan Meerut , 1998

3. Goldstein, Poole &Saiko, Classical Mechanics, Pearson Education 2002

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UNIT -7 Eulerian angles, Motion in a Non-Inertial Frame

Structure of the Unit

7.0 Objectives

7.1 Introduction

7.2 Eulerian Angles

7.3 Free motion of a symmetrical top

7.4 Euler's equations

7.5 Illustrative Examples

7.6 Motion in a Non-Inertial Frame of Reference

7.7 Illustrative Examples

7.8 Self Learning Exercise

7.9 Illustrative Examples

7.10 Summary

7.11 Glossary

7.12 Answers to Self Learning Exercise

7.13 Exercise

7.14 Answers to Exercise

References and Suggested Readings

7.0 Objectives

Our objectives in this chapter are :

- To express kinetic energy of rotation of a rigid body in terms of Eulerian angles.
- To discuss the precessional motion of a symmetrical top
- To derive the Euler's equations of motion
- Motion in a non-inertial framed of reference

- Motion in a rotating frame of reference and Coriolis force.

  Lagrangian function in a rotating frame.

7.1 Introduction

In this chapter we consider motion of rigid bodies, which require six generalized coordinates for the specification of their configurations. A general displacement of a rigid body can be considered to be a combination of translations and rotations. Of the six independent coordinates there are used to specify the rotational motion. These are the three angles that describe the orientation of the body axes with respect to the space-fixed axes. Though several choices are available, Euler's angles are the most commonly used ones. In this chapter we specify the orientation of the axes x_1, x_2, x_3 in the moving system of coordinates relative to the fixed system X, Y, Z. In this chapter we also obtain the relation connecting the inertial acceleration of the particle and its acceleration relative to the rotating frame. We derive some important formulae that describe the law of transformation of energy when we change to a uniformly rotating frame.

7.2 Eulerian Angles

The motion of a rigid body can be described by means of the ***three co-ordinates of its centre of mass and any three angles which determine the orientation*** of the axes x_1, x_2, x_3 in the moving system of Coordinates relative to the fixed system X, Y, Z.

These angles may often be conveniently taken as what are called "Eulerian angles".

Since we are here interested only in the angles between the coordinates axes, we may take the origins of two system to coincide.

The moving x_1x_2 plane intersects the fixed $X - Y$ plane in some line ON, called the line of nodes.

This line is evidently perpendicular to both the Z –axis and the x_3 axis. We take its positive direction as that of the vector product $\hat{z} \times \hat{x}_3$.

We take as the quantities defining the position of the axes x_1, x_2, x_3 relative to the axes X, Y, Z the-

* Angle θ between Z and x_3 axes.
* The angle ϕ between X-axis and ON.
* and the angle Ψ between the x_1 axis and ON.

The angles ϕ and Ψ are measured round the Z and x_3 axes respectively in the direction given by the Cork Screw Rule.

The angles θ takes values from 0 to π , and ϕ and Ψ from 0 to 2π.

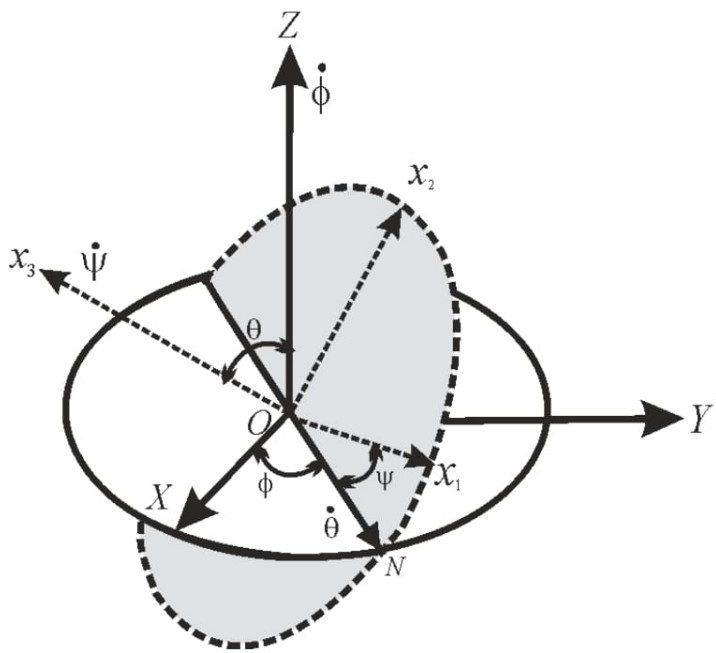


Figure 7.1

Let us now express the components of the angular velocity vector $\overrightarrow{\Omega}$ along the moving axes x_1, x_2, x_3 in term of Eulerian angles and their derivatives.

To do this, we must find the components only those axes of the angular velocities $\dot{\theta}, \dot{\phi}, \dot{\Psi}$.

$$\dot{\theta}_1 = \dot{\theta} \cos \Psi,$$
$$\dot{\theta}_2 = \dot{\theta} \sin \Psi,$$

$$\dot{\theta}_3 = 0 \{\because \dot{\theta}\cos(\Psi + 90) = -\dot{\theta}\sin\Psi\}$$

The angular velocity $\dot{\phi}$ is along Z-axis ;

$$\therefore \dot{\phi}_3 = \dot{\phi}\cos\theta \text{ (along } x_3\text{–axis) and } \dot{\phi}\sin\theta \text{ in the } x_1\, x_2 \text{ plane.}$$

$$\dot{\phi}_1 = \dot{\phi}\sin\theta\cos(90 - \Psi) = \dot{\phi}\sin\theta\sin\Psi$$

$$\dot{\phi}_2 = \dot{\phi}\sin\theta\sin(90 - \Psi) = \dot{\phi}\sin\theta\sin\Psi$$

Finally the angular velocity $\dot{\Psi}$ is along the x_3-axes.

Collecting the components along each axis, we have

$$\Omega_1 = \dot{\phi}\sin\theta\sin\Psi + \dot{\theta}\cos\Psi$$

$$\Omega_2 = \dot{\phi}\sin\theta\cos\Psi - \dot{\theta}\sin\Psi$$

$$\Omega_3 = \dot{\phi}\cos\theta + \dot{\Psi} \qquad (1)$$

If the axes x_1, x_2, x_3 are taken to be the principal axes of inertia of the body, the rotational K.E. in terms of Eulerian angles :

for a symmetrical top ($I_1 = I_2 \neq I_3$), a simple reduction gives :

$$T_{rot} = \frac{1}{2} I_1 \left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) + \frac{1}{2} I_3(\dot{\phi}\cos\theta + \dot{\Psi})^2 \qquad (2)$$

7.3 Free Motion of a Symmetrical Top

We take z-axis of the fixed system of coordinates in the direction of constant angular momentum $\vec{M}$ of the top.

The x_3 axis of the moving system is along the axis of the top;

Let x_1 axis coincide with the line of nodes at the instant considered.

Then $M_1 = I_1\Omega_1 = I_1\dot{\theta} \qquad (\because \Psi = 0)$

$$M_2 = I_1\Omega_2 = I_1\dot{\phi}\sin\theta$$

$$M_3 = I_3\Omega_3 = I_3(\dot{\phi}\cos\theta + \dot{\Psi})$$

Since x_1-axis is perpendicular to Z –axis ($\because x_1$ is along line of node)

$$\therefore M_1 = 0, M_2 = M\sin\theta, M_3 = M\cos\theta$$

$$M_1 = I_1\Omega_1 = I_1\dot{\theta}$$

$$\text{or } 0 = I_1\dot{\theta} \quad \therefore \dot{\theta} = 0$$

$$M_2 = I_1\Omega_2 = I_1\dot{\phi}\sin\theta$$

or $M_2 = M\sin\theta = I_1\dot{\phi}\sin\theta \qquad \therefore\ M = I_1\dot{\phi}$

$$\theta = constant$$

$$and\ \ I_3\left(\dot{\phi}\,cos\theta + \dot{\Psi}\right) = M\cos\theta$$

$\theta = constant$ i.e. the angle between the axis of top and the direction of $\vec{M}$ is constant.

The second equation gives the angular velocity of precession $\dot{\phi} = \frac{M}{I_1}$

Finally, the third equation gives the angular velocity with which the top rotates about its own axis :

$$\Omega_3 = \frac{M\cos\theta}{I_3}$$

7.4 Euler's Equations

The equations of motion $\frac{d\vec{P}}{dt} = \vec{F}$ as $\frac{d\vec{M}}{dt} = \vec{K}$ relate to the fixed system of coordinates.

The simplest relation between the components of the rotational angular momentum $\vec{M}$ of a rigid body and the components of the angular velocity occurs, however, in the moving system of coordinates whose axes are the principal axes of inertia.

In order to use this relation, we must first transform the equations of motion to the moving coordinates x_1, x_2, x_3.

Let : $\frac{d\vec{A}}{dt}$: rate of change of any vector $\vec{A}$ w.r.t. the fixed system of coordinates.

If the vector $\vec{A}$ does not change in the moving system its rate of change in the fixed system is due only to the rotation, so that $\frac{d\vec{A}}{dt} = \vec{\Omega}\times\vec{A}$.

The formulae are valid for any vector.

In the general case, the R.H.S. includes also the rate of change of the vector $\vec{A}$ w.r.t. the moving system:

$$\frac{d\vec{A}}{dt} = \frac{d'\vec{A}}{dt} + \vec{\Omega}\times\vec{A} \qquad (1)$$

Using this general formulae , we can immediately write equation of motion in the form :

$$\frac{d'\vec{P}}{dt} + \vec{\Omega} \times \vec{P} = \vec{F} \quad , \quad \frac{d'\vec{M}}{dt} + \vec{\Omega} \times \vec{M} = \vec{K} \tag{2}$$

Since the differentiation w.r.t. time is here performed in the moving system of coordinates, we can take the components of equations (2) along the axes of that system, putting $\left(\frac{d'\vec{P}}{dt}\right)_1 = \frac{dP_1}{dt}$,...., $\left(\frac{d'\vec{M}}{dt}\right)_1 = \frac{dM_1}{dt}$ where 1, 2, 3 denote components along the axes x_1, x_2, x_3. If μ is the mass of the body, then we replace $\vec{P} = \mu\,\vec{V}$ obtain

$$\begin{aligned}
\mu\left(\frac{dV_1}{dt} + \Omega_2 V_3 - \Omega_3 V_2\right) &= F_1 \\
\mu\left(\frac{dV_2}{dt} + \Omega_3 V_1 - \Omega_1 V_3\right) &= F_2 \\
\mu\left(\frac{dV_3}{dt} + \Omega_1 V_2 - \Omega_2 V_1\right) &= F_3
\end{aligned} \tag{3}$$

If the x_1, x_2, x_3 axes are the principal axes of inertia.

We can put

$$M_1 = I_1\Omega_1, M_2 = I_2\Omega_2, M_3 = I_3\Omega_3 :$$

$$I_1\frac{d\Omega_1}{dt} + \Omega_2 I_3\Omega_3 - \Omega_3 I_2\Omega_2 = K_1$$

$$or \quad I_1\frac{d\Omega_1}{dt} + \Omega_2\Omega_3(I_3 - I_2) = K_1$$

Similarly

$$I_2\frac{d\Omega_2}{dt} + (I_1 - I_3)\,\Omega_3\Omega_1 = K_2 \tag{4}$$

and $$I_3\frac{d\Omega_3}{dt} + (I_2 - I_1)\,\Omega_1\Omega_2 = K_3$$

These are Euler's equations.

In free rotation, $\vec{K} = 0$,

so that Euler's equations become :

$$\frac{d\Omega_1}{dt} + (I_3 - I_2)\frac{\Omega_2\Omega_3}{I_1} = 0$$

$$\frac{d\Omega_2}{dt} + (I_1 - I_3)\frac{\Omega_3\Omega_1}{I_2} = 0 \qquad (5)$$

$$\frac{d\Omega_3}{dt} + (I_2 - I_1)\frac{\Omega_1\Omega_2}{I_3} = 0$$

As an example, consider for rotation of a symmetrical top :

$\because\ I_1 = I_2$

We find $\dot{\Omega}_3 = 0, \quad \therefore\ \Omega_3 = Constant$

We then write the first two equations :

$$\dot{\Omega}_1 = -\omega\Omega_2$$

$$where\ \omega = \Omega_3\left(\frac{I_3 - I_1}{I_1}\right) = constant.$$

$$\dot{\Omega}_2 = \omega\Omega_1 \qquad (6)$$

Multiplying the eq.(6) by i and adding $\dot{\Omega}_1$:

$$\frac{d}{dt}(\Omega_1 + i\Omega_2) = +i\omega\,[\Omega_1 + i\Omega_2]$$

$$\therefore\ \Omega_1 + i\Omega_2 = Aexp(i\omega t)$$

$$\Omega_1 = A\cos\omega t,\ \Omega_2 = A\sin\omega t \qquad (7)$$

This result shows that the component of the angular velocity perpendicular to the axis of the top rotates with an angular velocity ω, remaining of constant magnitude

$$A = \sqrt{\Omega_1^2 + \Omega_2^2}\,.$$

Since the component Ω_3 along the axis of the top is also constant, we conclude that the vector $\vec{\Omega}$ rotates uniformly with angular velocity ω about the axes of the top, remaining unchanged in magnitude.

On account of the relations

$M_1 = I_1\Omega_1, M_2 = I_2\Omega_2, M_3 = I_3\Omega_3$ between the components of $\vec{\Omega}$ and $\vec{M}$,the angular momentum vector $\vec{M}$ evidently executes a similar motion w.r.t. the axis of the top.

This description is naturally only a different view of motion already discussed previously, where it was referred to the fixed system of coordinates.

In particular the angular velocity of the vector $\vec{M}$ (the z-axis) about the x_3–axis is, in terms of Eulerian angles, the same as the angular velocity $= -\dot{\Psi}$

$$\because \ \Omega_3 = \dot{\phi}\cos\theta + \dot{\Psi}$$

$$\because \ I_3 = \left(\dot{\phi}\cos\theta + \dot{\Psi}\right) = M\cos\theta$$

$$\therefore \ \dot{\Psi} = \frac{M\cos\theta}{I_3} - \dot{\phi}\cos\theta$$

$$= M\cos\theta\left(\frac{1}{I_3} - \frac{1}{I_1}\right)$$

$$\because \ I_1\dot{\phi} = M$$

$$or \ -\dot{\Psi} = \frac{\Omega_3(I_3 - I_1)}{I_1} \text{(in aggregate with (6))}$$

7.5 Illustrative Examples

Example 7.1: Reduce to quadratures the problem of the motion of a heavy symmetrical top whose lowest point is fixed.

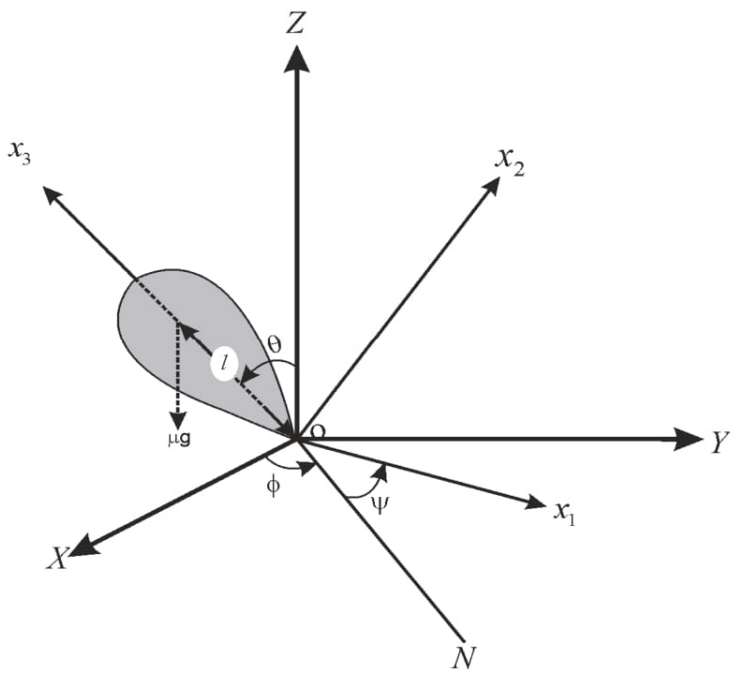


Figure 7.2

Sol. We take the common origin of the moving and fixed systems of coordinates at the fixed point O of the top and Z-axis vertical.

The Lagrangian of the top in a gravitational field is :

$$L = \frac{1}{2}(I_1 + \mu l^2)\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) + \frac{1}{2} I_3(\dot{\Psi} + \dot{\phi}\cos\theta)^2 - \mu g l \cos\theta$$

Where μ is the mass of the top end l the distance from its fixed point to the centre of mass.

The Coordinates Ψ and ϕ are cyclic. Hence we have two integrals of the motion.

Hence we have two integrals of the motion :

$$P_\Psi = \frac{\partial L}{\partial \dot{\Psi}} = I_3\left(\dot{\Psi} + \dot{\phi}\cos\theta\right) = constant \equiv M_3 \quad (1)$$

$$P_\phi = \frac{\partial L}{\partial \dot{\phi}}$$

$$= (I'_1 \sin^2\theta + I_3 \cos^2\theta)\dot{\phi} + I_3\dot{\Psi}\cos\theta = const. = M_z \quad (2)$$

where $I'_1 = (I_1 + \mu l^2)$

Where, the quantities P_Ψ and P_ϕ are the components of the rotational angular momentum about O along the x_3 and z-axis respectively.

The energy

$$E = \frac{1}{2} I'_1\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) + \frac{1}{2} I_3\left(\dot{\Psi} + \dot{\phi}\cos\theta\right)^2 + \mu g l \cos\theta \quad is\ also\ conserved \quad (3)$$

From (1) and (2) we found :

$$\dot{\phi} = \frac{(M_z - M_3\cos\theta)}{I'_1 \sin^2\theta} \quad (4)$$

$$\dot{\Psi} = \frac{M_3}{I_3} - \cos\theta \ \frac{M_z - M_3\cos\theta}{I'_1 \sin^2\theta} \quad (5)$$

Eliminating $\dot{\phi}$ and $\dot{\Psi}$ from the equation (3) by means of (4) and (5) we obtain :

$$E' = \frac{1}{2} I'_1\dot{\theta}^2 + U_{eff}(\theta)$$

Where $E' = E - \frac{M_3^2}{2I_3} - \mu g l$

$$U_{eff} = \frac{(M_z - M_3\cos\theta)^2}{2I'_1 \sin^2\theta} - \mu g l (1 - \cos\theta)$$

Thus we have :

$$t = \int \frac{d\theta}{\sqrt{\frac{2\left[E' - U_{eff}(\theta)\right]}{I'_1}}} \tag{7}$$

This is an elliptic integral. The angles Ψ and ϕ are then expressed in terms of θ by means of integrals obtained from equations (4) and (5).

The range of variation of θ during the motion is determined by the condition $E' \geq U_{eff}(\theta)$.

The function $U_{eff}(\theta)$ tends to ∞ $(if\ M_3 \neq M_z)$

When θ tends to 0 or π and has a minimum between these values.

Hence the equation $E' = U_{eff}(\theta)$ has two roots, which determine the limiting values $\theta_1\ and\ \theta_2$ of the inclination of the axis of the top to the vertical.

When θ varies from $\theta_1\ to\ \theta_2$ the derivative $\dot{\phi}$ changes sign if and only if the difference $M_z - M_3 \cos\theta$ changes sign in that range of θ.

If it does not change sign, the axis of the top precesses monotonically about the vertical at the same time oscillating up and down.

The latter oscillation is called ***mutation.***

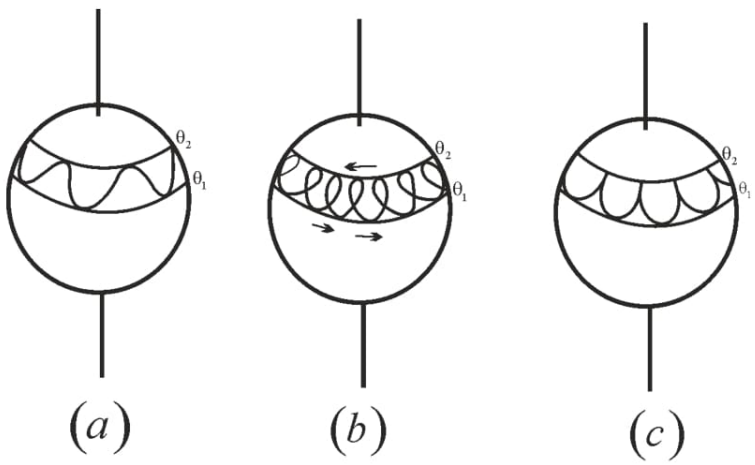


Figure 7.3 (a),(b),(c)

(see fig) Where the curve shows the track of the axis on the surface of a sphere whose centre is at the fixed point of the top.

If $\dot{\phi}$ changes sign, the direction of precession is opposite on the two limiting circles and so the axis of the top describes loops as it moves round the vertical $figure(b)$.

Finally if one of θ_1, θ_2 is a zero of $M_z - M_3 \cos\theta$, $\dot{\phi}$ and $\dot{\theta}$ vanish together on the corresponding limiting circle and the path of the axis is of the kind shown in fig (c).

7.6 Motion in a Non-Inertial Frame of Reference

We have always used inertial frame of reference so far :

Lagrangian in inertial frame

$$L_0 = \frac{1}{2}\, m\, v_0^2 - U \qquad (1)$$

and the corresponding equation of motion

$$m\, \frac{d\vec{v}_0}{dt} = -\frac{\partial U}{\partial \vec{r}} \quad (\because ma = F) \qquad (2)$$

subscript'0' denotes inertial frame. (true in inertial frame K_0)

- In noninertial frame, the principle of least action is valid, hence equation of motion remains of same form

Lagrange's equations.

$\frac{d}{dt}\left(\frac{\partial L}{\partial \vec{v}}\right) = \frac{\partial L}{\partial \vec{r}}$ are likewise valid $\left(\because \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0\right)$

But the Lagrangian is no longer of the form (1)

To derive it Let $'$: frame of reference moves with a translational velocity $\overrightarrow{V}(t)$ with respect to K_0 inertial frame

Let $\overrightarrow{v'}$ = Velocity of the particle with respect to K' frame

$\vec{v}_0$= Velocity of the particle with respect to K_0 frame,

Thus $\overrightarrow{v}_0 = \overrightarrow{v'} + \overrightarrow{V}$

Putting this into eq.(1)

$$L' = \frac{1}{2}\, m\left(v'^2 + 2\,\overrightarrow{v'}.\overrightarrow{V} + V^2\right) - U$$

$$L' = \frac{1}{2} m v'^2 + m \overrightarrow{v'} . \overrightarrow{V} + \frac{1}{2} m V^2 - U$$

$$\because m \overrightarrow{V}(t) . \overrightarrow{v'} = m \overrightarrow{V} . \frac{d\overrightarrow{r'}}{dt} = \frac{d}{dt} \left(m \overrightarrow{V} . \overrightarrow{r'} \right) - m \overrightarrow{r'} . \frac{d\overrightarrow{V}}{dt}$$

$$\therefore L' = \frac{1}{2} m v'^2 - m\overrightarrow{W}(t) . \overrightarrow{r'} - U$$

$\overrightarrow{W}$ =Translational acceleration of the frame K'

$$\therefore m \frac{d\overrightarrow{v'}}{dt} = -\frac{\partial U}{\partial \overrightarrow{r'}} - m \overrightarrow{W}(t)$$

Thus an accelerated translational motion of a frame of reference is equivalent as regards its effect on the equation of motion of a particle ,to the application of a uniform field of force equal to mass of after particle multiplied by the acceleration $\vec{w}$ in the direction opposite to this acceleration.

Let us now bring in a further frame of reference K ,whose origin coincides with that of K' but which rotates relative to K' with angular velocity $\vec{\Omega}(t)$.

Thus K executes both a translational and rotational with relative to K_0.Now we have

$$\boxed{\vec{v}' = \vec{v} + \vec{\Omega} \times \vec{r}}$$

Thus

$$L = \frac{1}{2} m v^2 + m \overrightarrow{v} . \vec{\Omega} \times \overrightarrow{r} + \frac{1}{2} m \left(\vec{\Omega} \times \overrightarrow{r} \right)^2 - m\overrightarrow{W} . \overrightarrow{r} - U$$

$$dL = m \overrightarrow{v} . d\overrightarrow{v} + m \, d\overrightarrow{v} . \vec{\Omega} \times \overrightarrow{r} - m\overrightarrow{v} . \left(\vec{\Omega} \times d\vec{r} \right) + m \left(\vec{\Omega} \times \overrightarrow{r} \right) . \left(\vec{\Omega} \times d\vec{r} \right) - m\overrightarrow{W} . d\overrightarrow{r} - \frac{\partial V}{\partial \overrightarrow{r}} . d\overrightarrow{r}$$

$$= m\overrightarrow{v} . d\overrightarrow{v} + m d\overrightarrow{v} . \vec{\Omega} \times \overrightarrow{r} + m \, d\overrightarrow{r} . \overrightarrow{v} \times \vec{\Omega} + m \left(\vec{\Omega} \times \vec{r} \right) \times \vec{\omega} . d\overrightarrow{r} - m\overrightarrow{W} . d\,\overrightarrow{r} - \left(\frac{\partial U}{\partial \overrightarrow{r}} \right) . d\overrightarrow{r}$$

$$\therefore \frac{\partial \mathrm{L}}{\partial \vec{\mathrm{v}}} = \mathrm{m}\overrightarrow{\mathrm{v}} + \mathrm{m} \, \vec{\Omega} \times \mathrm{r}$$

$$\frac{\partial L}{\partial \overrightarrow{r}} = m\overrightarrow{v} \times \vec{\Omega} + m \left(\vec{\Omega} \times \overrightarrow{r} \right) \times \vec{\Omega} - m\overrightarrow{W} - \frac{\partial U}{\partial \vec{r}}$$

$$\therefore m\frac{d\vec{v}}{dt} = -\frac{\partial U}{\partial \vec{r}} - m\vec{W} + m\vec{r} \times \dot{\vec{\Omega}} + 2m\vec{v} \times \vec{\Omega}$$
$$+m\vec{\Omega} \times (\vec{r} \times \vec{\Omega})$$

Inertia Forces:

$m\vec{r} \times \dot{\vec{\Omega}}$: *Force due to nonuniformity of te rotation*

$2m\vec{v} \times \vec{\Omega}$: **Coriolis**

$m\vec{\Omega} \times (\vec{r} \times \vec{\Omega})$: **centrifugal force**

$$\boxed{\text{Coriolis Force} = -2m(\vec{\Omega} \times \vec{v})}$$

$$\boxed{\text{Centrifugal Force} = -m\vec{\Omega} \times (\vec{\Omega} \times \vec{r})}$$

Now Consider pure rotation motion (with No translation)

$$\vec{W} = 0, \vec{\Omega} = constant$$
$$L = \frac{1}{2}m v^2 + m\vec{v}.(\vec{\Omega} \times \vec{r}) + \frac{1}{2}m(\vec{\Omega} \times \vec{r})^2 - U$$
$$\therefore m\frac{d\vec{v}}{dt} = -\frac{\partial U}{\partial \vec{r}} + 2m\vec{v} \times \vec{\Omega} + m\vec{\Omega} \times (\vec{r} \times \vec{\Omega})$$
$$\because \vec{p} = \frac{\partial L}{\partial \vec{v}} = m\vec{v} + m\vec{\Omega} \times \vec{r}$$
$$\varepsilon = \vec{p}.\vec{v} - L = \frac{1}{2}m v^2 - \frac{1}{2}m(\vec{\Omega} \times \vec{r})^2 + U$$
$$\text{Here } -\frac{1}{2}m(\vec{\Omega} \times \vec{r})^2 = centrifugal\ Potential\ Eenergy$$

The rotation of the frame simply adds to the energy a term depending only on the coordinates of the particle and proportional to the square of angular velocity.

Let $\vec{v}$ = velocity of the particle relative to uniformly rotating frame.

The velocity $\vec{v}$ of the particle relative to the uniform rotation frame of reference is relates to its velocity$\vec{v_0}$ relative to inertial frame K_0 is

$$\vec{v}_0 = \vec{v} + \vec{\Omega} \times \vec{r}$$

The momentum $\vec{p}$ of the particle in the frame K is

$$\vec{p} = m\vec{v} + m\vec{\Omega} \times \vec{r} = m\vec{v_0}$$

$\overrightarrow{p}_0$ = (same as in frame K_0)

The angular momentum $\overrightarrow{M_0} = \overrightarrow{r} \times \overrightarrow{p}_0$ and $\overrightarrow{M} = \overrightarrow{r} \times \overrightarrow{p}$ are likewise equal.

The energy of the particle in the two frames are not the same however.

Since $E = \frac{1}{2} mv^2 + \frac{1}{2} m (\vec{\Omega} \times \overrightarrow{r})^2 + U$

$$= \frac{1}{2} m (\overrightarrow{v_0} - \vec{\Omega} \times \overrightarrow{r})^2 - \frac{1}{2} m (\vec{\Omega} \times \overrightarrow{r})^2 + U$$

$$= \frac{1}{2} mv^2 + \frac{1}{2} (\vec{\Omega} \times \overrightarrow{r})^2 - m \overrightarrow{v_0} . (\vec{\Omega} \times \overrightarrow{r}) - \frac{1}{2} m (\vec{\Omega} \times \overrightarrow{r})^2 + U$$

$$= \frac{1}{2} m \overrightarrow{v_0} . \overrightarrow{v_0} + U - m \overrightarrow{v_0} . (\vec{\Omega} \times \overrightarrow{r})$$

$$= E_0 - \vec{\Omega} . \overrightarrow{r} \times m \overrightarrow{v_0}$$

$$E = E_0 - \vec{\Omega} . \vec{M}$$

This formula gives the law of transformation of energy when we change to a uniformly rotating frame.

7.7 Illustrative Examples

Example 7.2 A body of mass 2kg is projected with velocity $\vec{v}$ from a frame of reference which has angular velocity $\vec{\omega}$ Here $\vec{v} = 2\hat{i} + 3\hat{j} + 4\hat{k}$ m/sec $\vec{\omega} = -3\hat{i} + 2\hat{j} - 5\hat{k}$ $rad/\sec$ Calculate the Coriolis force acting on the particle.

Sol. Coriolis force acting on the particle is given by

$$\text{Coriolis Force} = -2m(\vec{\omega} \times \vec{v})$$

$$\vec{F} = -2m(\vec{\omega} \times \vec{v})$$

$$\vec{F} = -2(2)\left(-3\hat{i} + 2\hat{j} - 5\hat{k}\right) \times \left(2\hat{i} + 3\hat{j} + 4\hat{k}\right)$$

$$\vec{F} = -4 \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -3 & 2 & -5 \\ 2 & 3 & 4 \end{vmatrix}$$

$$\vec{F} = -2(2)\left[\hat{i}(8+15) - \hat{j}(-12+10) + \hat{k}(-9-4)\right]$$

$$\vec{F} = -4\left[\hat{i}(23) - \hat{j}(-2) + \hat{k}(-13)\right]$$

$$\vec{F} = \left[92\hat{i} + 8\hat{j} + 53\hat{k}\right]$$

In magnitude $\left|\vec{F}\right| = \left[92^2 + 8^2 + 53^2\right]^{\frac{1}{2}}$ $\left|\vec{F}\right| = \left[92^2 + 8^2 + 53^2\right]^{\frac{1}{2}}$

$$\left|\vec{F}\right| = \left[8464 + 64 + 2809\right]^{\frac{1}{2}} \Rightarrow \left|\vec{F}\right| = \sqrt{11337}\ Newton$$

7.8 Self Learning Exercise

Very Short Answer type Questions

Q.1 Write down the expression for Coriolis force

Short Answer Type Questions

Q.2 Define the Euler's angles .

Q.3 Derive the Euler's equations of motion in terms of Euler's angles.

7.9 Illustrative Examples

Example 7.3 Find the deflection of a freely falling body from a vertical caused by the Earth's rotation, assuming the angular velocity of this rotation to be small,

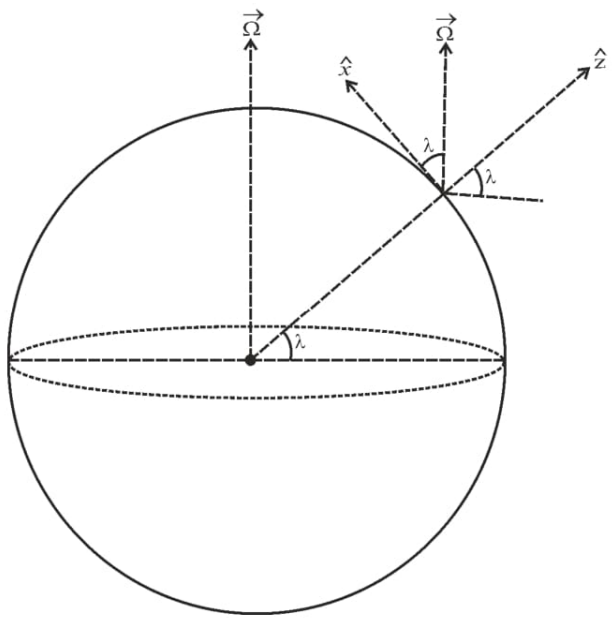


Figure 7.4

$$U = -m\vec{g}.\vec{r}$$

Neglecting the centrifugal force

Equation of motion

$$\dot{\vec{v}} = 2\vec{v} \times \vec{\Omega} + \vec{g} \tag{1}$$

To solve this equation, we make use of successive approx.

$$\vec{v} = \vec{v_1} + \vec{v_2}$$

$$\dot{\vec{v}}_1 = \vec{g} \qquad \therefore \ \vec{v_1} = \vec{g}t + \vec{v_0} \quad (\vec{v_0} : Initial\ velocity)$$

Putting these values in eq.(1)

$$\therefore \ \dot{\vec{v}}_1 + \dot{\vec{v}}_2 = 2\,(\vec{g}t + \vec{v_0}) \times \vec{\Omega} + \vec{g}$$

$$\dot{\vec{v}}_2 = 2\,\vec{v_1} \times \vec{\Omega}$$

$$= 2\,(\vec{g}t + \vec{v_0}) \times \vec{\Omega}$$

$$\dot{\vec{v}}_2 = 2t\,\vec{g} \times \vec{\Omega} + 2\,\vec{v_0} \times \vec{\Omega}$$

$$\therefore \ \vec{r} = \vec{h} + \vec{v_0} + \vec{g}\frac{t^2}{2} + \frac{2(\vec{g} \times \vec{\Omega})}{2} \times \frac{t^3}{3} + (\vec{v_0} \times \vec{\Omega})\frac{t^2}{2}$$

$$= \vec{h} + \vec{v_0}t + \frac{1}{2}\vec{g}t^2 + \frac{1}{3}t^3\,(\vec{g} \times \vec{\Omega}) + (\vec{v_0} \times \vec{\Omega})t^2 \tag{2}$$

where $\vec{h}$ is the initial radius vector.

Let z – axis be vertically upwards and x-axis towards the pole.

$$(\therefore \ g_x = g_y = 0, g_z = -g)$$

$$\Omega_x = \Omega\cos\lambda,$$

$$\Omega_y = 0,$$

$$\Omega_z = \Omega\sin\lambda$$

Putting $v_0 = 0,\ x = 0\ ,\ y = -\frac{1}{3}t^3\,g\Omega\cos\lambda$

$$\because t \approx \sqrt{\frac{2h}{g}}$$

We finally get $x = 0, y = -\frac{1}{3}\left(\frac{2h}{g}\right)^{3/2} g\,\Omega\cos\lambda$

-ve sign indicates eastward deflection.

Example 7.4: Determine the deflection from Coplanarity of the path of a particle thrown from the Earth's surface with velocity $\overrightarrow{v_0}$.

Sol. Let the xz-planes be such as to contain the velocity $\vec{v}_0$ (i.e. $\vec{v}_0 = (V_{0x}, o, V_{0z})$

The initial altitude h = 0

The lateral deviation is given by the expression derived in the previous problem.

$$\vec{r} = \vec{h} + \vec{v_0}\, t + \frac{1}{2}\vec{g}\, t^2 + \frac{1}{3}t^3\, \vec{g} \times \vec{\Omega} + t^2\, \vec{v_0} \times \vec{\Omega}$$

$$\therefore y = 0 + 0 + 0 + \frac{1}{3}t^3\,(g\Omega_x - g_x\Omega_z) + t^2(v_{0z}\Omega_x - v_{0x}\Omega_z)$$

$$y = \frac{1}{3}t^2\,(-g)\,\pi\cos\lambda - 0 + t^2\,(v_{0z}\,\pi\cos\lambda - v_{0x}\,\pi\sin\lambda)$$

$$\because 0 = v_{0z} - gt \qquad \therefore t \approx \frac{v_{0z}}{g} \times 2$$

$$y = \frac{1}{3}\,\frac{v_{0z}^3}{g^3}\,(-g)\Omega\cos\lambda + 4\,\frac{v_{0z}^2}{g^2}\,(v_{0z}\,\Omega\cos\lambda - v_{0x}\,\Omega\sin\lambda)$$

$$= 4\,\frac{v_{0z}^3}{g^2}\,\Omega\cos\lambda\left[-\frac{2}{3} + 1\right] - 4\,\frac{v_0 \times v_{0z}^2}{g^2}\,\Omega\sin\lambda)$$

$$= \frac{4}{3}\,\frac{v_{0z}^2}{g^2}\left\{\frac{1}{3}\,v_{0z}\,\Omega\cos\lambda - v_{0z}\,\Omega\sin\lambda\right\}$$

$$= \frac{4v_{0z}^2}{g^2}\left\{\frac{1}{3}\,v_{0z}\,\Omega_x - v_{0z}\,\Omega_z\right\}$$

Example 7.5: Determine the effect of the Earth's rotation on small oscillations off a pendulums (the problem of Foucault's pendulum)

Sol. Neglecting the vertical displacement of the pendulum as being a quantity of the second order of smallness ,we can regard the motion as taking place in the horizontal xy-plane.

Neglecting the terms in Ω^2 , we have the equations of motion.

$$m\dot{x} = -mg\theta + 2m(\vec{v} \times \vec{\Omega})_x$$

$$\ddot{x} = -\frac{g}{l}\,x + 2\left[v_y\Omega_z - v_z\Omega_y\right]$$

$\ddot{x} + \omega^2 x = 2\Omega_z\dot{y} - 0$ (we neflect vertical displacement so $v_z = 0$)

Similarly $\ddot{y} + \omega^2 = 2[v_z x - z\Omega_z]$

$$\ddot{y} + yx = -2\dot{x}\,\Omega_z \tag{2}$$

$$\frac{d}{dt}(\dot{x} + 2i\dot{y}) + \omega^2(\dot{x} + 2y) = -2i\Omega_z(\dot{x} + i\dot{y})$$

Let $x + iy = \xi$

$$\ddot{\xi} + 2i\,\Omega_z\,\dot{\xi} + \omega^2.\xi = 0$$

$$\xi = e^{\lambda t}$$

$$\lambda^2 + 2i\,\Omega_z\lambda + \omega^2 = 0$$

$$\therefore\ \lambda = -2i\Omega_z \pm \frac{\sqrt{-4\Omega_z^2 - 4\omega^2}}{2}$$

$$\lambda = -i\Omega_z \pm \sqrt{\Omega_z^2 + \omega^2}$$

$$\approx -i\Omega_z \pm i\,\omega$$

$$\varepsilon = A_1 e^{(-i_z + i\,\omega)t} + A_2 e^{(-i_z - i\,\omega)t}$$

$$= e^{-i_z t}\{A_1 e^{i\omega t} + A_2 e^{-i\omega t}\}$$

$$x + iy = e^{-i_z t}\{x_0 + iy_0\}$$

Where the functions $x_0(t), y_0(t)$ give the path of the pendulum when the Earth's rotation is neglected.

The effect of this rotation is therefore to twin the path about the vertical with angular velocity $\Omega_z = \omega\sin\lambda$.

$$\mathrm{T} = \frac{2\pi}{\omega\,\sin\lambda}$$

7.10 Summary

In this chapter we have discussed rotation of a rigid body in terms of Eulerian angles. We have derived kinetic energy of rotation in terms of Eulerian angles. We have also discussed "free rotation" of a symmetric top along with precessional motion of the top. We have also discussed the motion of a body in a non-inertial frame and discussed the effects of "inertia forces" on the motion of the body. We have explained the eastward deflection of a body falling freely from a height.

7.11 Glossary

Integrals of the Motion: During the motion of a mechanical system, the '*2s*' quantities q_i and $\dot{q}_i$ (i = 1, 2, ... *s*) which specify the state of the system vary with time. There exist, however, functions of these quantities whose values remain constant during the motion, and depend only on the initial conditions. Such functions are called "integrals of motion".

Translational: Movement of a body from one point of space to another such that every point of the body moves in the same direction and over the same distance, without any rotation ,reflection, or change in size.

***Coplanarity*:** something happen in same plane

7.12 Answers to Self Learning Exercise

Ans.1: $-2m\left(\vec{\omega}\times\vec{v}\right)$

7.13 Exercise

Section A:Very Short Answer Type Questions

Q.1 The angular velocity of precession $\dot{\phi}$ of a symmetrical top is

(A) $\dot{\phi}=\frac{M}{I}$ (B) $\frac{M\cos\theta}{I_3}$ (C) $\frac{M}{I_3}$ (D) $\frac{M\cos\theta}{I}$

Q.2 Euler's equations relate to the

(A) fixed system of coordinates (B) moving system of coordinates

(C) arbitrary frame of reference (D) inertial frame of reference

Q.3 The law of transformation of energy when we change to a uniformly rotating frame is (symbol have usual meaning).

(A)$E = E_0$ (B) $E=\vec{\Omega}\,.\,\vec{M}$

(C) $E=\vec{E_0}-\vec{\Omega}\,.\,\vec{M}$ (D) $E=\vec{E_0}+\vec{\Omega}\,.\,\vec{M}$

Q.4 Deflection of a freely falling body from a vertical can be explained on the basis of

(A)Coriolis force acting on the body caused by Eearth's rotations

(B)centrifugal force

(C)Gravitational force

(D)Frictional forces

Q.5 Write down the expression for Centrifugal force.

Section B:Short Answer Type Questions

Q.6 Calculate the Coriolis force acting on an object of mass 0.5Kg moving southwards with a horizontal velocity of 200m/s at 30^0 N latitude on the earth.

Section C:Long Answer Type Questions

Q.7 Discuss the theory of symmetric top moving under gravity.

Q.8 A body initially at rest is dropped from at the height h .Assume that height h is negligible in comparison to radius of earth R. Prove that after a time t the object is deflected east of vertical by $\frac{1}{2}\omega g t^3 \sin\lambda$

,where ω is the angular velocity of the earth which is taken as constant and λ is the colatitudes of the place.

7.14 Answers to Exercise

Ans.1:A **Ans.2:**B

Ans.3:C **Ans.4:A**

Ans.5: $\text{Centrifugal Force} = -m\vec{\Omega}\times\left(\vec{\Omega}\times\vec{r}\right)$

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UNIT-8
The Canonical Equations,Poisson Brackets

Structure of the Unit

8.0 Objectives

8.1 Introduction

8.2 The Canonical Equations

8.3 Hamiltonian for a single particle in Cartesian cylindrical and spherical coordinates

8.4 Illustrative Examples

8.5 Self Learning Exercise-I

8.6 Illustrative Examples

8.7 Possion's Brackets : (P.B.)

8.8 Jacobi's Identity

8.9 Poission's Theorem

8.10 Self Learning Exercise-II

8.11 Summary

8.12 Glossary

8.13 Answers to Self Learning Exercises

8.14 Exercise

8.15 Answers to Exercise

References and Suggested Readings

8.0 Objectives

Our objectives in this chapter are :

1. To derive Hamilton's canonical equations making use of the "Legendre's transformations".
2. To derive equation of motion in terms of Poisson bracket.
3. To state and prove Poisson's theorem.

8.1 Introduction

In this chapter we derive the equations of motion in terms of generalized coordinates and momenta of the system. In Lagrangian formulation we derive equations of motion in terms of generalized coordinates and generalized velocities. However in many applications in physics it is convenient to work in terms of coordinates and momenta.

In this chapter we shall transform equations of motion from the set of variables $(q, \dot{q})$ to (q, p). This is known as "Hamiltonian mechanics". We derive Hamilton's canonical equations of motion. We introduce a function of dynamical variables in terms of "Poisson brackets".

8.2 The Canonical Equations

The formulation of the laws of mechanics in terms of the Lagrangian/Lagrangian equations presupposes that the mechanical state of the system is described by specifying its generalized coordinates and velocities.

This is not the only possible mode of description, however.

A number of advantages, especially in the study of certain general problems of mechanics, attach to a description in terms of the generalized coordinates and momenta of the system.

The question therefore arises of the form of the equations of motion corresponding to that formulation of mechanics.

The passage from one set of independent variables to another can be effected by means of what is called in mathematics "Legendre's transformation".

In the present case the transformation is as follows :

The total differential of the Lagrangian can be written as:

$$\boxed{dL = \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i}$$

$$= \sum_i \dot{p}_i dq_i + \sum_i p_i d\dot{q}_i \qquad \left[\because \frac{\partial L}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \dot{p}_i \right]$$

$$= \sum_i \dot{p}_i dq_i + d\sum_i (p_i \dot{q}_i) - \sum_i \dot{q}_i dp_i$$

$$\text{or } d\left(\sum_i p_i\dot{q}_i - L\right) = -\sum_i \dot{p}_i dq_i + \sum_i \dot{q}_i dp_i$$

$$\text{or } dH = -\sum_i \dot{p}_i dq_i + \sum_i \dot{q}_i dp_i$$

where H = Hamilton's function $\boxed{H = \sum_i p_i\dot{q}_i - L}$

$$\therefore \boxed{\dot{p}_i = -\frac{\partial H}{\partial q_i},\ \dot{q}_i = \frac{\partial H}{\partial p_i}}$$

These are the required equations of motion and are called Hamilton's equations. (also called canonical equations).

They form a set of *2s* first-order differential equations for the *2s* unknown functions $p_i(t)$ and $q_i(t)$, replacing the *s* second order equations in the Lagrangian treatment .The time derivative of the Hamiltonian is

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \sum_i \frac{\partial H}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial H}{\partial p_i}\dot{p}_i$$

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \qquad \left(\because \dot{q}_i = +\frac{\partial H}{\partial p_i}, \dot{p}_i = -\frac{\partial H}{\partial q_i}\right)$$

In particular if the Hamiltonian does not depend explicitly on time, then $\frac{\partial H}{\partial t} = 0$ ***, and we have the law of conservation of energy.***

As well as the dynamical variables $q, \dot{q}$ *or* q, p the Lagrangian and the Hamiltonian involve various parameters which relate to the properties of the mechanical system itself.

Let λ be one such parameter, regarding it as a variable.

We write

$$dL = \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial \lambda} d\lambda$$

$$= -\sum_i \dot{p}_i dq_i + \sum_i p_i d\dot{q}_i + \frac{\partial L}{\partial \lambda} d\lambda$$

$$= -\sum_i \dot{p}_i dq_i + d\left(\sum_i p_i\dot{q}_i\right) - \sum_i \dot{q}_i dp_i + \frac{\partial L}{\partial \lambda} d\lambda$$

$$\text{or } dH = \sum_i \dot{p}_i dq_i + \sum_i \dot{q}_i dp_i - \frac{\partial L}{\partial \lambda} d\lambda$$

$$\therefore \left(\frac{\partial H}{\partial \lambda}\right)_{p,q} = -\left(\frac{\partial L}{\partial \lambda}\right)_{\dot{q},q}$$

Which relates the derivatives of the Lagrangian and the Hamiltonian with respect to the parameter λ.

The suffixes to the derivatives show the quantities which are to be kept constant in the differentiation.

Let $L = L_0 + L'$ and the corresponding addition to the Hamiltonian be

$$H = H_0 + H'$$

Then $(\mathrm{H}')_{p,\mathrm{q}} = -(\mathrm{L}')_{\mathrm{q},\dot{\mathrm{q}}}$

Also $\boxed{\left(\frac{\partial H}{\partial t}\right)_{q,p} = -\left(\frac{\partial L}{\partial t}\right)_{\dot{q},q}}$

8.3 Hamiltonian for a Single Particle in Cartesian, Cylindrical and Spherical Coordinates

As we know that the Lagrangian for a single particle in Cartesian ,Cylindrical and Spherical coordinates is given by

$$\boxed{L = \frac{1}{2} m(\dot{\mathrm{x}}^2 + \dot{\mathrm{y}}^2 + \dot{\mathrm{z}}^2) - \mathrm{U(x,y,z)}} \quad (1)$$

$$\boxed{L = \frac{1}{2} m(\dot{\mathrm{r}}^2 + r^2\dot{\phi}^2 + \dot{\mathrm{z}}^2) - \mathrm{U(r},\phi,\mathrm{z})} \quad (2)$$

$$\boxed{L = \frac{1}{2} m(\dot{\mathrm{r}}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) - \mathrm{U(r},\theta,\phi)} \quad (3)$$

Eq. (1) is for Cartesian, Eq. (2) for cylindrical and Eq. (3) for spherical coordinates. We can now write the Hamiltonian H(p,q) in Cartesian coordinates as

$$\mathrm{H} = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + U(x,y,z) \quad (4)$$

In cylindrical coordinates we write

$$\mathrm{p}_r = \frac{\partial L}{\partial \dot{r}} = \frac{1}{2} m.2\dot{r}$$

or $\dot{r} = \frac{\mathrm{p}_r}{m}$.

Similarly $\boxed{p_\phi = \frac{\partial L}{\partial \dot{\phi}}} = mr^2\dot{\phi}$

or $\dot{\phi} = \frac{\mathrm{p}_\phi}{mr^2}$, and $\dot{z} = \frac{\mathrm{p}_z}{m}$.

Expressing kinetic energy in terms of momenta $p_r, p_\phi \; and \; p_z$

we find

$$\mathrm{H} = \frac{1}{2m}\left(p_r^2 + \frac{p_\phi^2}{r^2} + p_z^2 \right) + U(r,\phi,z) \tag{5}$$

In spherical coordinates we find

$\frac{\mathrm{p}_r}{m} = \dot{r}$, $p_\phi = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta}$, and $p_\phi = mr^2 \sin^2\theta\dot{\phi}$. We find

$$\boxed{\mathrm{H} = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta} \right) + U(r,\theta,\phi)} \tag{6}$$

8.4 Illustrative Examples

Example. 1: Obtain the equation of motion for Simple pendulum using Hamilton's equations.

Sol. The kinetic energy of the bob of simple pendulum is

$$\boxed{T = \frac{1}{2} ml^2\dot{\theta}^2}$$

The potential energy of the system

$$V = mgl\left(1 - \cos\theta\right)$$

Lagrangian of the system

$$L = T - V$$

$$= \frac{1}{2} ml^2 \dot{\theta}^2 - mgl\left(1 - \cos\theta\right) \tag{1}$$

Thus $L = T - V$

$$= \frac{1}{2} ml^2 \dot{\theta}^2 - mgl\left(1 - \cos\theta\right)$$

gives $p_\theta = \frac{\partial L}{\partial \dot{\theta}} = ml^2 \dot{\theta}$

The Hamiltonian of the system

$$H = \sum p_i \dot{q}_i - L$$

$$= p_\theta \dot{\theta} - L$$

$$= ml^2 \dot{\theta}^2 - \left\{ \frac{1}{2} ml^2 \dot{\theta}^2 - mgl\left(1 - \cos\theta\right) \right\}$$

$$= \frac{1}{2} ml^2 \dot{\theta}^2 + mgl\left(1 - \cos\theta\right) \tag{3}$$

$$= T + V,$$

In this case H is the total energy of the system.

Now putting eq. (2) into eq. (3), we get

$$H = \frac{1}{2} ml^2 \left(\frac{p_\theta}{ml^2} \right)^2 + mgl\left(1 - \cos\theta\right)$$

gives

$$\left.\begin{aligned} \frac{\partial H}{\partial p_\theta} &= \frac{p_\theta}{ml^2} \\ \frac{\partial H}{\partial \theta} &= mgl \sin\theta. \end{aligned}\right] \tag{4}$$

Hamilton's equations of motion for this system is

$$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ml^2} \tag{5}$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = -mgl \sin\theta. \tag{6}$$

Putting the value of $\dot{p}_\theta$ from eq. (5) into eq. (6), we get

$$ml^2\ddot{\theta} = -mgl\sin\theta$$

or $$\ddot{\theta} + \frac{g}{l}\sin\theta = 0$$

Example 2: Obtain the equation of motion for Linear Harmonic Oscillator using Hamilton's equations.

Sol. Linear Harmonic Oscillator (system)is conservative and constraint is independent of time, Therefore Hamiltonian is equal to the total energy of the system. The Lagrangian is given by

$$L = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

or $$\frac{\partial L}{\partial \dot{x}} = \frac{\partial T}{\partial \dot{x}} = p = m\dot{x}$$

gives $$\dot{x} = p/m$$

We can represent Hamiltonian in terms of momentum,

$$H = T + V$$

$$= \frac{1}{2}m\left(p/m\right)^2 + \frac{1}{2}kx^2$$

$$= p^2/2m + \frac{1}{2}kx^2$$

Equation of motion are given as

$$\left.\begin{aligned}\dot{p} &= -\frac{\partial H}{\partial x} = -kx \\ \dot{x} &= \frac{\partial H}{\partial p} = p/m\end{aligned}\right]$$

From last equation,

$$\ddot{x} = \dot{p}/m = -kx/m$$

which gives $$m\ddot{x} + kx = 0$$

Above equation represents the equation of motion of a simple pendulum

Example 3: Obtain the equation of motion for compound pendulum using Hamilton's equations.

Sol. The Lagrangian for a compound pendulum can be obtained as Kinetic energy

$$\boxed{T=\frac{1}{2}I\dot{\theta}^2}$$

Potential energy $V=-mgl\cos\theta$

Therefore $L=\frac{1}{2}I\dot{\theta}^2+mgl\cos\theta$

Then $p_\theta=\frac{\partial L}{\partial\dot{\theta}}=I\dot{\theta}$

The Hamiltonian is

$$\begin{aligned}
&= \sum p_i\dot{q}_i - L\\
&= p_\theta\dot{\theta}-L\\
&= I\dot{\theta}.\dot{\theta}-\frac{1}{2}I\dot{\theta}^2-mgl\cos\theta\\
&= \frac{1}{2}I\dot{\theta}^2-mgl\cos\theta\\
&= \frac{1}{2}I\left(\frac{p_\theta}{I}\right)^2-mgl\cos\theta\\
&= \frac{p_\theta^2}{2I}-mgl\cos\theta \qquad (2)\\
&= T+V
\end{aligned}$$

Thus above system is conservative in nature.

The Hamilton's equations of motion for θ and p_θ are

$$\left.\begin{aligned}\dot{\theta}&=\frac{\partial H}{\partial p_\theta}\\ \dot{p}_\theta&=-\frac{\partial H}{\partial\theta}\end{aligned}\right] \qquad (3)$$

From equation (2), we get

$$\frac{\partial H}{\partial p_\theta}=\frac{p_\theta}{I},\quad \frac{\partial H}{\partial p_\theta}=mgl\ \sin\theta$$

Putting these is eqs. (3), we have

$$\dot{\theta}=\frac{p_\theta}{I}$$

and $$\dot{p}_\theta = -mgl\sin\theta$$

From eq. (4) & eq. (5) ,we get

$$I\ddot{\theta}=-mgl\sin\theta$$

or $$\ddot{\theta}+\frac{mgl}{I}\sin\theta=0$$

Above equation represents the equation of motion of compound pendulum.

Example 4: Obtain the equation of motion for Two dimensional Isotropic Harmonic Oscillator using Hamilton's equations in Cartesian as well as in polar co-ordinates.

Sol. Two dimensional Isotropic Harmonic Oscillator

We shall discuss the equations of motion in Cartesian as well as in polar co-ordinates:

(a) In Cartesian Co-ordinates:

The Lagrangian of the Two dimensional Isotropic Harmonic Oscillator is

$$L=T-V$$

$$=\frac{1}{2}m\left(\dot{x}^2+\dot{y}^2\right)-\frac{1}{2}k\left(x^2+y^2\right) \qquad (1)$$

Gives

and
$$\left.\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} = m\dot{x} \qquad or \qquad \dot{x}=\frac{p_x}{m} \\ p_y &= \frac{\partial L}{\partial \dot{y}} = m\dot{y} \qquad or \qquad \dot{y}=\frac{p_y}{m} \end{aligned}\right] \qquad (2)$$

The Hamiltonian H is given by

$$H=\sum_i p_i\dot{q}_i - L$$

$$= p_x\dot{x}+p_y\dot{y}-\frac{1}{2}m\left(\dot{x}^2+\dot{y}^2\right)+\frac{1}{2}k\left(x^2+y^2\right)$$

$$= \frac{p_x^2}{m} + \frac{p_y^2}{m} - \frac{1}{2}\left(\frac{p_x^2}{m} + \frac{p_y^2}{m}\right) + \frac{1}{2}k\left(x^2 + y^2\right)$$

$$= \frac{1}{2}\left(p_x^2 + p_y^2\right) + \frac{1}{2}k\left(x^2 + y^2\right)$$

Gives

$$\left.\begin{aligned} \frac{\partial H}{\partial p_x} &= \frac{p_x}{m}, \quad \frac{\partial H}{\partial p_y} = \frac{p_y}{m} \\ \frac{\partial H}{\partial x} &= kx, \quad \frac{\partial H}{\partial y} = ky \end{aligned}\right] \tag{3}$$

Using eq.(3)the Hamilton's equations are

$$\left.\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p_x} = \frac{p_x}{m} \\ \dot{p}_x &= -\frac{\partial H}{\partial x} = -kx \end{aligned}\right] \tag{4}$$

and

$$\left.\begin{aligned} \dot{y} &= \frac{\partial H}{\partial p_y} = \frac{p_y}{m} \\ \dot{p}_y &= -\frac{\partial H}{\partial y} = -ky \end{aligned}\right] \tag{5}$$

From eqs. (4) and (5), we have

$$\left.\begin{aligned} m\ddot{x} + kx = 0 \\ m\ddot{y} + ky = 0 \end{aligned}\right]$$

which are required equations.

8.5 Self Learning Exercise-I

Q.1 Prove the relation

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}$$

Q.2 What is meant by generalized coordinates? Derive Hamilton's canonical equation of motion in generalized coordinates and explain the significance of Hamiltonian.

Q.3 If the Lagrangian of a system is given be

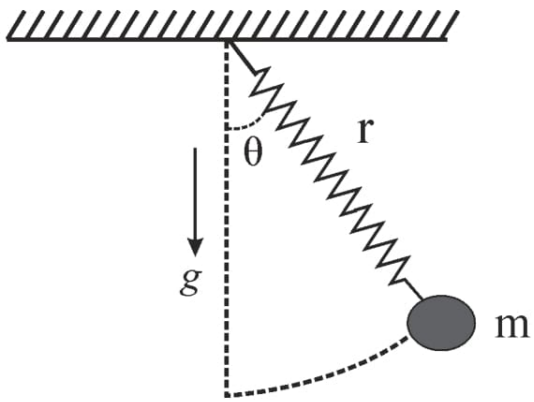
$$L(q_j, \dot{q}_j) = \frac{1}{2}c_1\dot{q}_j^2 + \frac{1}{2}c_2 q_j^2$$

where c_1 and c_2 are constants, obtain the Hamiltonian.

8.6 Illustrative Examples

Example5: Find the equations of motion of a pendulum bob suspended by a spring and allowed to swing in a vertical plane.

Sol.



Taking reference of potential energy at the support, then the potential energy is

$$U = -\int \vec{F}.\vec{r} = -mgr\cos\theta + \text{due to extension of spring}$$

or $U = -mgr\cos\theta + \frac{1}{2}k(r - r_0)^2$ where r_0 is the unstretched length of spring.

Therefore

$$H = T + U$$

$$= \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) - mgr\cos\theta + \frac{1}{2}k(r - r_0)^2$$

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \tag{1}$$

$$-\dot{p}_r = \frac{\partial H}{\partial r} = -\frac{p_\theta^2}{mr^3} - mg\cos\theta + k(r - r_0)$$

$$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{mr^2}$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = -[\text{mgrsin}\,\theta] \qquad (2)$$

From (1) and (2) we get

$$\text{m}\ddot{r} - \text{mr}\dot{\theta}^2 - mg\cos\theta + k(r - r_0) = 0$$

$$mr^2\ddot{\theta} + 2mr\dot{r}\dot{\theta} + mgr\sin\theta = 0,$$

which are the desired equations of motion.

8.7 Poisson's Brackets : (P.B.)

Let *f(p, q, t)* be some function of coordinates, momenta and time. Its total time derivative is

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_k \left(\frac{\partial f}{\partial q_k}\dot{q}_k + \frac{\partial f}{\partial p_k}\dot{p}_k \right)}$$

Substituting

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

$$\Rightarrow \frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_k \left(\frac{\partial f}{\partial q_k}.\frac{\partial H}{\partial p_k} - \frac{\partial f}{\partial p_k}\frac{\partial H}{\partial q_k} \right)$$

$$\Rightarrow \boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + [H, f]}$$

Where $[H, f] = \sum_k \left(\frac{\partial H}{\partial p_k}\frac{\partial f}{\partial q_k} - \frac{\partial H}{\partial q_k}\frac{\partial f}{\partial p_k} \right) \equiv$ Poisson's Bracket of H and f

These functions of the dynamical variables which remain constant during the motion of the system are, as we know ,called "Integrals of Motion".

The condition for the quantity f to be an integral of the motion $\left(\frac{df}{dt} = 0 \right)$ can be written as

$$\frac{\partial f}{\partial t} + [H, f] = 0$$

If the integral of the motion is not explicitly dependent on time, then

$$[H, f] = 0$$

i.e. ***the Poisson bracket of the integral and the Hamiltonian must be zero.***

For any quantities f and g the P.B. is defined analogous

$$\boxed{[f, g] \equiv \sum_k \left(\frac{\partial f}{\partial p_k} \cdot \frac{\partial g}{\partial q_k} - \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} \right)}$$

Important Points :-

- $\boxed{[f, g] = -[g, f]}$
- $\boxed{[\mathrm{f}, \mathrm{c}] = 0}$ where c is some constant
- $[f_1 + f_2, f] = [f_1 g] + [f_2, g]$
- $[f_1 + f_2, f] = f_1[f_2 g] + f_2[f_1, g]$
- $\boxed{\frac{\partial}{\partial t}[f, g] = \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right]}$
- $[f, q_k] = \frac{\partial f}{\partial p_k}$,

  $[f, \mathrm{p}_k] = -\frac{\partial f}{\partial q_k}$
- $\boxed{[\mathrm{q}_i, q_k] = 0}$, $\boxed{[\mathrm{p}_i, p_k] = 0}$, $\boxed{[\mathrm{p}_i, q_k] = \delta_{ik}}$

8.8 Jacobi's Identity

The Jacobi's identity is the following relation

$$\boxed{[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0} \qquad (1)$$

Proof. As we know by the definition of Poisson's Bracket [f, g], that it is a linear homogeneous function of the first derivatives of f and g.

Hence the bracket $[h,(f, g)]$ is a large homogeneous function of the second derivatives of f and g. The left hand side of (1) is therefore a linear homogeneous function of the second derivatives of all three functions f, g, h.

Let $D_1(\phi) = [\mathrm{g}, \phi]$, $D_2(\phi) = [\mathrm{h}, \phi]$ then

$$[g,[h,f]] = \mathrm{D}_1 D_2 f$$

and $[h,[f,g]] = -[h,[g,f]] = -D_2 \mathrm{D}_1 f$

Therefore $[g,[h,f]] + [h,[f,g]] = [g,[h,f] - [h,[g,f]]$

$$= \mathrm{D}_1 D_2 f - D_2 \mathrm{D}_1 f$$

where $\mathrm{D}_1 = \sum_k \xi_k \frac{\partial}{\partial x_k}$, $\mathrm{D}_2 = \sum_k \eta_k \frac{\partial}{\partial x_k}$

Where ξ_k and η_k are functions of the variables $x_1, x_2, ...$ Then

$$\mathrm{D}_1 D_2 = \sum_{k,l} \xi_k \frac{\partial}{\partial x_k}\left(\eta_l \frac{\partial ....}{\partial x_l}\right)$$

$$= \sum_{k,l} \xi_k \frac{\partial \eta_l}{\partial x_k}\frac{\partial}{\partial x_l} + \sum_{k,l} \xi_k \eta_l \frac{\partial^2}{\partial x_k \partial x_l}$$

$$\mathrm{D}_2 D_1 = \sum_{k,l} \eta_k \frac{\partial}{\partial x_k}\left(\xi_k \frac{\partial ....}{\partial x_l}\right) = \sum_{k,l} \eta_k \xi_l \frac{\partial^2}{\partial x_k \partial x_l} + \sum_{k,l} \eta_k \frac{\partial \xi_l}{\partial x_k}\frac{\partial}{\partial x_l}$$

$$\therefore \mathrm{D}_1 D_2 - \mathrm{D}_2 D_1 = \sum_{k,l}\left\{\xi_k \frac{\partial \eta_l}{\partial x_k} - \eta_k \frac{\partial \xi_l}{\partial x_k}\right\}\frac{\partial}{\partial x_l}$$

Therefore we note that $\mathrm{D}_1 D_2 - \mathrm{D}_2 D_1$ is again an operator involving only single differentiations. Thus terms in the second derivatives of f on the left hand side of (1) cancel and, since the same is of course true of g and h, the whole expression is identically zero.

8.9 Poisson's Theorem

An important property of the Poisson's bracket is that if f and g are two integrals of motion, their Poisson's bracket is also an integral of motion:

$$[f,g] = \text{constant}$$

This is Poisson's theorem.

Proof : The proof is very simple if f and g do not depend explicitly on the time. Putting h = H in

Jacobi's identity, we obtain

$$[\mathrm{H},[\mathrm{f},g]] + [\mathrm{f},[g,\mathrm{H}] + [g,[\mathrm{H},f]] = 0$$

Hence if $[\mathrm{H}, g]=0$ and $[\mathrm{H}, \mathrm{f}]=0$ then

$[H,[f, g]=0,$ i.e. $[\mathrm{f}, \mathrm{g}]=\text{constant}$,

which is the required result.

If the integrals f and g of the motion are explicitly time-dependent, we put

$$\begin{aligned}\frac{d}{dt}[\mathrm{f}, \mathrm{g}] &= \frac{\partial}{\partial t}[f, g]+[H,[f, g]] \\ &= \left[\frac{\partial f}{\partial t}, g\right]+\left[f, \frac{\partial g}{\partial t}\right]-[f,[g, \mathrm{H}]]-[\mathrm{g},[\mathrm{H}, \mathrm{f}]] \\ &= \left[\frac{\partial f}{\partial t}+[H, f], g\right]+\left[f, \frac{\partial g}{\partial t}+[H, g]\right] \\ &= \left[\frac{df}{dt}, g\right]+\left[f, \frac{dg}{dt}\right],\end{aligned}$$

which evidently proves Poisson's theorem.

Example 6: Show that $[\Phi, M_z]=0$, where Φ is any function, spherically symmetrical about the origin, of the coordinates and momentum of a particle.

Sol. Such a function Φ can depend on $r^2, \mathrm{p}^2, \vec{r}.\vec{p}$. Hence

$$\frac{\partial \Phi}{\partial \vec{r}}=\frac{\partial \Phi}{\partial(\mathrm{r}^2)}.2\vec{r}+\frac{\partial \Phi}{\partial(\vec{p}.\vec{r})}\vec{p}$$

and similarly for

$$\frac{\partial \Phi}{\partial \vec{p}}=\frac{\partial \Phi}{\partial(\mathrm{p}^2)}.2\vec{p}+\frac{\partial \Phi}{\partial(\vec{p}.\vec{r})}\vec{r}$$

We write

$$\begin{aligned}[\Phi, M_z] &= [\Phi, \mathrm{xp}_y-\mathrm{yp}_x] \\ &= [\Phi, \mathrm{xp}_y]-[\Phi, \mathrm{yp}_x] \\ &= [\Phi, \mathrm{x}]\mathrm{p}_y+\mathrm{x}[\Phi, \mathrm{p}_y]-[\Phi, \mathrm{y}]\mathrm{p}_x-[\Phi, \mathrm{p}_x]\mathrm{y} \\ &= \frac{\partial \Phi}{\partial \mathrm{p}_x}\mathrm{p}_y+x\left(-\frac{\partial \Phi}{\partial y}\right)-\frac{\partial \Phi}{\partial \mathrm{p}_y}p_x+\frac{\partial \Phi}{\partial x}y \\ &= \frac{\partial \Phi}{\partial p^2}.2p_x\,\mathrm{p}_y+\frac{\partial \Phi}{\partial(\vec{p}.\vec{r})}.\mathrm{x}\,p_y-x\left(\frac{\partial \Phi}{\partial r^2}2y+\frac{\partial \Phi}{\partial(\vec{p}.\vec{r})}p_y\right)\end{aligned}$$

$$-p_x\left(\frac{\partial\Phi}{\partial p^2}2p_y+\frac{\partial\Phi}{\partial(\mathrm{p.r})}y\right)+\left(\frac{\partial\Phi}{\partial r^2}.2x+\frac{\partial\Phi}{\partial(\mathrm{p.r})}p_x\right)y$$
$$=0$$

8.10 Self Learning Exercise-II

Q.1 Lagrangian $L=\frac{1}{8}m\left[(\xi+\eta)\left(\frac{\dot{\xi}^2}{\xi^2}+\frac{\dot{\eta}^2}{\eta^2}\right)+4\xi\eta\dot{\varphi}^2\right]+\frac{1}{8}k(\xi+\eta)^2$

where k is constant. Then which of the following the conserved quantity will be in the system

(a) $(m+k)(\dot{\xi}+\dot{\eta})$ (b) $\mathrm{m}(\xi+\eta)\left(\frac{\dot{\xi}}{\xi^2}+\frac{\dot{\eta}}{\eta^2}\right)$

(c) $m\left(\frac{\dot{\xi}^2}{\eta^2}+\frac{\dot{\eta}^2}{\xi^2}\right)$ (d) $m\xi\eta\dot{\varphi}$

Q.2 Prove the relation

$$[f_1f_2,g]=f_1[f_2,g]+f_2[f_1,g]$$

Q.3 Deduce the relation :

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+[\mathrm{H,f}]$$

Q.4 Determine the Poisson Brackets (PBs) from the components of $\overrightarrow{M}$.

8.11 Summary

In this chapter we have derived canonical equations of motion in terms of generalized coordinates and generalized momenta. This mode of description of a dynamical system is advantageous in many applications of quantum and relativistic mechanics.

8.12 Glossary

Integral of motion :During the motion of a mechanical system, the '*2s*' quantities q_i and $\dot{q}_i$ (i = 1, 2, ... *s*) which specify the state of the system vary with time. There exist, however, functions of these quantities whose values remain constant

during the motion, and depend only on the initial conditions. Such functions are called "integrals of motion".

Isotropic: having same properties in every direction

Homogeneous*:* in mathematics containing terms all of the same degree.

8.13 Answers to Self Learning Exercises

Answers to Self Learning Exercise-I

Ans.3 : $L = T - U$, So $U = -\frac{1}{2}c_2 q_j^2$

$$T = \frac{1}{2}\dot{q}_j^2$$

Expressing $\dot{\mathrm{q}}_j$ in terms of p_j by using the relation

$$\mathrm{p}_j = \frac{\partial L}{\partial \dot{q}_j} = \frac{1}{2}c_1 . 2\dot{q}_j$$

$$\dot{q}_j = \frac{\mathrm{p}_j}{c_1}$$

Thus $H(q_j, p_j) = \frac{1}{2}c_1 \frac{\mathrm{p}_j^2}{c_1^2} + \frac{1}{2}c_2 q_j^2$

$$H = \frac{\mathrm{p}_j^2}{2c_1} + \frac{1}{2}c_2 q_j^2$$

Answers to Self Learning Exercise-II

Ans.1 (a)

Ans.4 : A direct calculation gives

$$\begin{aligned}
[\mathrm{M}_x, \mathrm{M}_y] &= [\mathrm{M}_x, zp_x - \mathrm{x}\, p_z] \\
&= [\mathrm{M}_x, z\, p_x] - [\mathrm{M}_x, xp_z] \\
&= \mathrm{z}[\mathrm{M}_x, \mathrm{p}_x] + p_x[\mathrm{M}_x, z] - [\mathrm{M}_x, x]\mathrm{p}_z - [\mathrm{M}_x, \mathrm{p}_z]\mathrm{x} \\
&= 0 + \mathrm{p}_x\, y - 0 - \mathrm{p}_y\, x \\
&= -[x\,\mathrm{p}_y - y\,\mathrm{p}_x] = -M_z
\end{aligned}$$

Similarly

$$[M_y, M_z] = -M_x \; ; [M_z, M_x] = -M_y$$

8.14 Exercise

Q.1 A dynamical system with two degrees of freedom, has generalized coordinates q_1 and q_2 and kinetic energy

$$T = \lambda \dot{q}_1 \dot{q}_2$$

If the potential energy is $V(q_1, q_2) = 0$, the correct form of the Hamiltonian for this system is

(A) $\frac{p_1 p_2}{\lambda}$ (B) $\lambda \dot{q}_1 \dot{q}_2$

(C) $(p_1 \dot{q}_1 + p_2 \dot{q}_2)/2$ (D) $(p_1 q_2 + p_2 q_1)/2$

Q.2 The Lagrangian for a simple pendulum is given by

$$L = \frac{1}{2} m l^2 \dot{\theta}^2 - mgl(1 - \cos\theta)$$

Which of the options is correct about Hamilton's equations

(A) $\dot{p}_\theta = -mgl \sin\theta \; ; \dot{\theta} = \frac{p_\theta}{ml^2}$ (B) $\dot{p}_\theta = +mgl \sin\theta \; ; \dot{\theta} = \frac{p_\theta}{ml^2}$

(C) $\dot{p}_\theta = -m\ddot{\theta} \; ; \; \dot{\theta} = \frac{p_\theta}{m}$ (D) $\dot{p}_\theta = -\frac{g}{l}\theta \; ; \dot{\theta} = \frac{p_\theta}{ml}$

Q.3 Prove the relations

$$[p_i, p_k] = 0 \quad ; [p_i, q_k] = \delta_{ik}$$

Q.4 State and prove Poisson's theorem

Q.5 Prove the relation

$$\frac{\partial}{\partial t}[f, g] = \left[\frac{\partial f}{\partial t}, g\right] + \left[f, \frac{\partial g}{\partial t}\right]$$

Q.6 Prove Jacobi's identity

Q.7 Prove the relations

(a) $[f, q_k] = \frac{\partial f}{\partial p_k}$ (b) $[f, p_k] = -\frac{\partial f}{\partial q_k}$ (c) $[f, p_k] = -\frac{\partial f}{\partial p_k}$

Q.8 Prove the relation

$$\left(\frac{\partial H}{\partial t}\right)_{q,p} = -\left(\frac{\partial L}{\partial t}\right)_{\dot{q},q}$$

Q.9 Determine the Poisson's Bracket formed from the Cartesian components of the momentum $\vec{p}$ and angular momentum $\vec{M} = \vec{r} \times \vec{p}$ of a particle.

Q.10 What is Legendre transformation? Using Legendre transformation obtain Hamilton's equations of motion from Lagrange's equation of motion.

Q.11 Lagrangian of anharmonic oscillator of unit mass is

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}\omega^2 x^2 - \alpha x^3 + \beta x \dot{x}^2 ,$$

where α and β are constants. Find the Hamiltonian and deduce the canonical equations of motion.

Q.12 $L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2\left[1+\left(\frac{df}{dx}\right)^2\right] - mgf(x)$, for a bead of mass m, sliding smoothly along a wire of shape z =f(x), z-axis and x-axis being respectively horizontal and vertical. Find the corresponding Hamiltonian.

Q.13 Derive Hamilton's equations of motion for a system of particles . Hence write down the equations of motion of a particle in a central force field in space.

Q.14 The Lagrangian for a system can be written as $L = a\dot{x}^2 + b\frac{\dot{y}}{x} + c\dot{x}\dot{y} + fy^2\dot{x}\dot{z} + g\dot{y} - k\sqrt{x^2+y^2}$ Where *a, b, c f, g* and *k* are constants .

What is the Hamiltonian? What quantities are conserved?

Q.15 A dynamical system has the Lagrangian

$$L = \dot{q}_1^2 + \frac{\dot{q}_2^2}{a + bq_1^2} + k_1 q_1^2 + k_2 \dot{q}_1 \dot{q}_2$$

where *a, b,* k_1, k_2 are constants.

Find the equations of motion in the Hamiltonian formulation.

8.15 Answers to Exercise

Ans.7: $[f, q_k] = \frac{\partial f}{\partial q_k}\frac{\partial q_k}{\partial q_k} - \frac{\partial f}{\partial q_k}.\frac{\partial q_k}{\partial p_k}$

$$= \frac{\partial f}{\partial p_k} \quad \left\{ \because \frac{\partial q_k}{\partial p_k} = 0 \ ; q_k, p_k \text{being independent variables} \right\}$$

Ans.9: $[\mathrm{M}_x, p_y] = -\frac{\partial}{\partial y} M_x = -\frac{\partial}{\partial y}\left(y, p_z - z p_y\right) = -p_z$

$[\mathrm{M}_x, p_z] = 0 \ ; [M_x, p_z] = p_y .$

The remaining brackets are obtained by permuting suffixes x, y, z.

Ans.11: $H = \dot{x}p - L$

$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x}(1 + 2\beta x)$$

So $\mathrm{H} = \frac{p^2}{2(1+2\beta x)} + \frac{1}{2} w^2 x^2 + \alpha x^3$

Equations of motion are

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{1+2\beta x}$$

$$\dot{p} = \frac{\partial H}{\partial x} = \beta \dot{x}^2 - w^2 x - 3\alpha x^2$$

Combining the above equations to get the equation of motion

$$(1+2\beta x)\ddot{x} + \beta \dot{x}^2 + w^2 x + 3\alpha x^2 = 0$$

Ans.12 : $\mathrm{H} = \frac{p^2}{2m\left[1 + \left(\frac{df}{dx}\right)^2\right]} + mgf(x)$

References and Suggested Readings

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UNIT-9

Action as a Function of the Coordinates , Canonical Transformations

Structure of the Unit

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9.0 Objectives

Our objectives in this chapter are :

(i) To introduce action S as a function of the coordinates and to show that $\frac{\partial S}{\partial q_i} = p_i$

(ii) To derive the relation : $dS = \sum_i p_i \, dq_i - H \, dt$.

(iii) To introduce Point transformations

(iv) To derive the generating functions of the Canonical transformation.

(v) To prove the invariance of Poisson's bracket under canonical transformation.

9.1 Introduction

In this chapter we will consider another aspect of action, regarding S as a quantity characterizing the motion along the actual path, and compare the values of S for paths having a common beginning, but passing through different points at a later time. In other words, we consider the action integral for the true path as a function of the coordinates at the other limit of integration.

9.2 The Action as a Function of the Coordinates

Action $\boxed{S = \int_{t_1}^{t_2} L dt}$

The change in the action from one path to neighboring path (if there is one degree of freedom) is given by the expression.

$$\delta S = \left[\frac{\partial L}{\partial \dot{q}}\delta q\right]_{t_1}^{t_2} + \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\right)\delta q dt$$

$$\therefore \delta S = p.\delta q$$

$$\delta S = \sum_i p_i \delta q_i$$

$$\frac{\partial S}{\partial q_i} = p_i$$

The action may similarly be regarded as an explicit function of time, by considering paths at a given instant t_1 and at given point $q^{(1)}$ and at given point $q^{(2)}$ at various times $t_2 = t$. The partial derivative $\frac{\partial S}{\partial t}$ thus obtained may be found by an appropriate variation of the integral.

It is simple, however to use formula $\frac{\partial S}{\partial q_i} = p_i$, proceeding as follows :

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \sum_i \frac{\partial S}{\partial q_i}\dot{q}_i = \frac{\partial S}{\partial t} + \sum_i p_i \dot{q}_i$$

$$\text{or } L - \sum_i p_i \dot{q}_i = \frac{\partial S}{\partial t}$$

$$\text{or } \boxed{\frac{\partial S}{\partial t} = -H}, \therefore dS = \frac{\partial S}{\partial q} dq + \frac{\partial S}{\partial t} dt$$

$$= pdq - Hdt$$

$$\therefore dS = \sum_i p_i dq_i - Hdt$$

Let us now suppose that the coordinates (and time) at the beginning motion, as well as at the end are variables. It is evident that the corresponding change in S will be given by the difference of the expression.

$$dS = \sum_i p_i^{(2)} dq^{(2)} - H^{(2)} dt^{(2)} - \sum_i p_i^{(1)} dq^{(1)} - H^{(1)} dt^{(1)}$$

9.3 Derivations of Hamilton's Canonical equations from Principle of Least Action

We know that $dS = \frac{\partial S}{\partial t} dt + \sum_i \frac{\partial S}{\partial q_i} dq_i$ (As action $S = S(q,t)$)

$$\text{or } \mathrm{dS} = -\mathrm{Hdt} + \sum_i p_i dq_i \qquad \left(-H = \frac{\partial S}{\partial t}, p_i = \frac{\partial S}{\partial q_i}\right)$$

$$S = \int \left[\sum_i p_i dq_i - Hdt \right]$$

We assume one degree of freedom, thus we write

$$S = \int [pdq - Hdt]$$

$$\delta S = \int \left[\delta p dq + pd(\delta q) - \left(\frac{\partial H}{\partial p}\right) \delta p dt - \left(\frac{\partial H}{\partial q}\right) \delta q dt \right]$$

$$= \int [\delta p dq] + [p \delta q] - \int dp.\delta q - \int \left(\frac{\partial H}{\partial p}\right) \delta p dt - \int \left(\frac{\partial H}{\partial q}\right) \delta q dt$$

$$\delta S = \int \left[\delta p dq - \left(\frac{\partial H}{\partial p}\right) \delta p dt \right] + [p \delta q]_{t_1}^{t_2} - \left[\int dp \delta q + \left(\frac{\partial H}{\partial q}\right) \delta q dt \right] = 0$$

Using $\delta q(t_1) = \delta q(t_2) = 0$, δS will be zero only if the integrands are zero and the variations δp and δq are arbitrary, we get

$$\frac{\partial H}{\partial p} = \frac{dq}{dt} \quad , \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

$$\boxed{\dot{q} = \frac{\partial H}{\partial p} \ , \ \dot{p} = -\frac{\partial H}{\partial q}}$$

9.4 Canonical Transformations

What are "point transformations"?

Lagrange's equations do not depend on the choice of the generalized coordinates q. In this sense the Lagrange's equations may be said to be invariant with respect to a transformation from the coordinates $q_1, q_2 \ldots\ldots$ to any other independent quantity $Q_1, Q_2 \ldots\ldots$ The new coordinates Q are function of q and we shall assume that they may explicitly depend on the time i.e.

$$\mathrm{Q}_i = Q_i(q,t) \qquad \text{(Point transformation)} \qquad (1)$$

Since Lagrange's equations are unchanged by the transformation (1), Hamilton's equations are also unchanged.

Hamilton's equations, however infact allow a much wider range of transformations. This is, of course, because in the Hamiltonian treatment the momenta p are variables independent of and on equal footing with coordinates q.

Hence the transformation may be extended to include all the 2*s* independent variables p and q.

$$\mathrm{Q}_i = Q_i(\mathrm{p},q,t), \ \ \mathrm{P}_i = P_i(p,q,t) \qquad (2)$$

This enlargement of the class of possible transformation is one of the important advantages of the Hamiltonian treatment. The equations of motion do not however, retain their canonical form under all transformations of the form (2). Let us derive the conditions which must be satisfied if the equations of motion in the new variables *P,Q* are to be of the form.

$$\dot{\mathrm{Q}}_i = \frac{\partial H'}{\partial \mathrm{P}_i}, \qquad \dot{\mathrm{P}}_i = -\frac{\partial H'}{\partial Q_i} \text{ with some Hamiltonian } H' = (P,Q) \qquad (3)$$

Among these transformation, there is a particularly important class called ***"Canonical transformations".***

The formula for canonical transformations can be obtained as follows:

Hamilton's equations can be derived from the principle of least action in the form : $\delta S = 0$

$$\text{or } \delta \int \left(\sum_i p_i . dq_i - H dt \right) = 0 \tag{4}$$

in which the variation is applied to all the coordinates and momenta independently. If the new variables P and Q also satisfy Hamilton's equations, the principle of least action must hold, i.e.

$$\delta \left(\sum_i P_i . dQ_i - H' dt \right) = 0 \tag{5}$$

The two forms (4) and (5) are certainly equivalent of their integrands are the same apart from the total differential of some function F of coordinates, momenta and time. The difference between the two integrals is then a constant, namely the difference of the values of F at the limits of integration, which does not affect the variation. Thus we will take

$$\sum_i p_i . dq_i - H dt = \sum_i P_i . dQ_i - H' dt + dF \tag{6}$$

Transformation which satisfy this condition are said to be canonical **;** Each transformation is characterized by a particular function F, called the "***generating functions***' of the transformation

Note : The canonical form of the equations of motion is preserved not only by the canonical transformations but also by transformations in which integrands in (4) and (5) differ by any constant factor. For example $P_i = ap_i, Q_i = q_i, H' = aH$ with any constant a. $\dot{P}_i = -\dfrac{\partial H'}{\partial Q_i}$ and $\dot{Q}_i = -\dfrac{\partial H'}{\partial P_i}$

Writing this relation is

$$dF = \sum_i p_i dq_i - \sum_i p_i dQ_i + (H' - H) dt$$

We see that

$$p_i = \frac{\partial F}{\partial q_i}, \qquad P_i = -\frac{\partial F}{\partial Q_i}, \quad H' = H + \frac{\partial F}{\partial t} \tag{7}$$

Here $F = F(q, Q, t)$ where F is known, formulae (7) give the relation between p,q and P,Q as well as the new Hamiltonian.

It may be convenient to express the generating function and in terms of q and Q but in terms of the old coordinate q and the new momenta P. To derive the formulae for canonical transformations in this case, we must effect the appropriate Legendre's transformation in (6) rewriting it

$$d\left(F + \sum_i P_i Q_i \right) = \sum_i p_i dq_i + \sum_i Q_i dP_i + (H' - H)dt$$

The new generating function $\phi(\mathrm{q}, P, \mathrm{t})$ gives

$$p_i = -\frac{\partial \phi}{\partial q_i}, \quad Q_i = -\frac{\partial \phi}{\partial P_i}, \quad H' = H + \frac{\partial \phi}{\partial t} \tag{8}$$

We can similarly obtain the formulae for canonical transformations involving generating functions which depend on the variables p and Q, or p and P.

The relation between the two Hamiltonian is always of the same form : $H' - H =$ partial derivatives of the generating function with respect to time.

In particular, if the generating function is independent of time, then $H' = H$ i.e. the new Hamiltonian is obtained by simply substituting for p, q in H their values in terms of the new variables P,Q.

The wide range of the canonical transformations in the Hamiltonian treatment deprives the generalized coordinates and momenta of a considerable part of then original meaning.

Thus is very clearly seen, for example from the transformation $Q_i = p_i$, $P_i = -q_i$, whose generating function is $F = \sum_i q_i Q_i$

The variables p and q in the Hamiltonian treatment are often called "***Canonically conjugate***" quantities.

The conditions relating such quantities can be expressed in terms of ***Poisson brackets***. To do this, we shall first prove a general theorem on the invariance of Poisson brackets with respect to canonical transformation. ***Let*** $[f, g]_{p,q}$ ***be the***

Poisson Bracket, for two quantities f and g in which the differentiation is with respect to the variables p and q and $[f,g]_{P,Q}$ ***that in which the differentiation is with respect to P and Q. Then***

$$[f,g]_{p,q} = [f,g]_{P,Q} \qquad \textbf{(9)}$$

The truth of this statement can be seen by direct calculation, using the formulae of the canonical transformation. It can also be demonstrated by the following argument :

"First of all, it may be noticed that the time appear as a parameter in the canonical transformations.

$\left\{ p_i = \frac{\partial F}{\partial q_i}, P_i = -\frac{\partial F}{\partial Q_i}, H' = H + \frac{\partial F}{\partial t}; or\ p_i = \frac{\partial \phi}{\partial q_i}, Q_i = \frac{\partial \phi}{\partial P_i}, H' = H + \frac{\partial \phi}{\partial t} \right\}$. It is therefore sufficient to prove

(a) for quantities which do not depend explicitly on time. Let us now formally regards g as the Hamiltonian of some fictitious system. Then by (1),

$$[f,g]_{p,q} = -\frac{df}{dt}\left(\because \frac{df}{dt} = \frac{\partial f}{\partial t} + [g,f], \quad \therefore [f,g] = -\frac{df}{dt} \right)$$

The derivative can depend only on the properties of the motion of the fictitious system, and not on the particular choice of variables. ***Hence the Poisson bracket [f,g] is unaltered by the passage from one set of canonical variable to another***.

Therefore we conclude

$$[Q_i, Q_k]_{p,q} = 0, [P_i, P_k]_{p,q} = 0, [P_i, Q_k]_{p,q} = \delta_{ik} \qquad (10)$$

These are the conditions, written in terms of Poisson brackets, which must be satisfied by the new variables if transformation $p,q \to P,Q$ is canonical.

9.5 Conditions for a Transformation to be canonical

➢ Poisson brackets conditions

$$\boxed{[Q_i, Q_k]_{p,q} = 0, [P_i, P_k]_{p,q} = 0, [P_i, Q_k]_{p,q} = \delta_{ik}}$$

➢ An Exact Differentiation condition

If the expression $\sum_j \left(P_j dQ_j - p_j dq_j \right)$

Or $\sum_j \left(p_j dq_j - P_j dQ_j \right)$ is an exact differential, then transformation is canonical.

We know that $\left(\sum_j p_j \dot{q}_j - H \right) - \left(\sum_j P_j \dot{Q}_j - H' \right) = \frac{dF}{dt}$

If generating function F does not include time then $H' = H + \frac{\partial F}{\partial t} = H$

then $\sum_j p_j \dot{q}_j - H - \sum_j P_j \dot{Q}_j + H' = \frac{dF}{dt}$

$$\sum_j p_j \dot{q}_j - \sum_j P_j \dot{Q}_j = \frac{dF}{dt}$$

$$\boxed{\sum_j p_j dq_j - \sum_j P_j dQ_j = dF}$$

Here dF is the exact differential of function F

➢ Bilinear Invariant Condition

If generating function F does not include time ,then bilinear form remains invariant i.e.

$$\boxed{\sum_j \left(\delta p_j dq_j - \delta q_j dp_j \right) = \sum_j \left(\delta P_j dQ_j - \delta Q_j dP_j \right)}$$

and transformation (q_j, p_j) set to (Q_j, P_j) set is canonical .

Note :

It is of interest to observe that the change in the quantities p,q during the motion may itself be regarded as series of canonical transformations. To see this

Let q_t, p_t be the values of the canonical variables of *t*, and $q_{t+\tau}, p_{t+\tau}$ their values at another time $t + \tau$. The latter are some function of the former (and involve τ as a parameters):

$$q_{t+\tau} = q(\mathrm{q}_t, \mathrm{p}_t, \mathrm{t}, \tau), p_{t+\tau} = (\mathrm{q}_t, \mathrm{p}_t, t, \tau)$$

If these formulae are regarded as a transformation from the variables $\mathrm{q}_t, \mathrm{p}_t$ to $q_{t+\tau}, p_{t+\tau}$, then this transformation is canonical.

This is evident from the expression

$dS = \sum\left(p_{t+\tau}dq_{t+\tau} - p_t dq_t\right) - (\mathrm{H}_{t+\tau} - H_t)dt$ for the differential of the action $S\left(q_{t+\tau}, q_t, t, \tau\right)$ taken along the true path, passing through the point q_t and $q_{t+\tau}$ at time t and $t+\tau$ for a given τ

$$\mathrm{dF} = \sum p_i dq_i - \sum P_i dQ_i - +(H' - H)dt$$

A comparison shows that $-S$ is the generating function of the transformation.

9.6 Illustrative Examples

Example1: For what values of the parameter α the following transformation is canonical?

$$Q = q\cos\alpha - p\sin\alpha$$
$$P = q\sin\alpha + p\cos\alpha$$

Sol. The transformation is canonically the Poisson bracket$[Q,P]_{q,p} = 1$ or

$$[\mathrm{P},\mathrm{Q}]_{p,q} = 1$$

We have

$$[\mathrm{P},\mathrm{Q}]_{p,q} = \frac{\partial P}{\partial p}\frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q}\frac{\partial Q}{\partial p}$$

$$[\mathrm{P},\mathrm{Q}]_{p,q} = \frac{\partial}{\partial p}(q\sin\alpha + p\cos\alpha)\frac{\partial}{\partial q}(q\cos\alpha - p\sin\alpha)$$
$$-\frac{\partial}{\partial q}(q\sin\alpha + p\cos\alpha)\frac{\partial}{\partial p}(q\cos\alpha - p\sin\alpha)$$
$$= (0+1.\cos\alpha)(1.\cos\alpha - 0) - (1.\sin\alpha + 0)(0 - 1.\sin\alpha)$$
$$= \cos\alpha.\cos\alpha - \sin\alpha(-\sin\alpha)$$
$$= \cos^2\alpha + \sin^2\alpha = 1$$

So, for all values of α, the given transformation is canonical.

Alternative

Bilinear Invariant Condition

Here $\sum_j\left(\delta P_j dQ_j - \delta Q_j dP_j\right)$

$$= \delta P\, dQ - \delta Q\, dP$$

$$
\begin{aligned}
&= \{\ \delta(q\sin\alpha + p\cos\alpha)d(q\cos\alpha - p\sin\alpha) \\
&\quad -\delta(q\cos\alpha - p\sin\alpha)d(q\sin\alpha + p\cos\alpha)\ \} \\
&= \{\ (\delta q\sin\alpha + \delta p\cos\alpha)(dq\cos\alpha - dp\sin\alpha) \\
&\quad -(\delta q\cos\alpha - \delta p\sin\alpha)(dq\sin\alpha + dp\cos\alpha)\ \} \\
&= \{\delta q\sin\alpha.dq\cos\alpha - \delta q\sin\alpha.dp\sin\alpha \\
&\quad + \delta p\cos\alpha.dq\cos\alpha - \delta p\cos\alpha.dp\sin\alpha \\
&\quad - \delta q\cos\alpha.dq\sin\alpha - \delta q\cos\alpha.dp\cos\alpha \\
&\quad + \delta p\sin\alpha.dq\sin\alpha + \delta p\sin\alpha.dp\cos\alpha\ \} \\
&= \{-\delta q\sin\alpha.dp\sin\alpha\ + \delta p\cos\alpha.dq\cos\alpha \\
&\quad - \delta q\cos\alpha.dp\cos\alpha + \delta p\sin\alpha.dq\sin\alpha +\ \} \\
&= \delta pdq(\cos^2\alpha + \sin^2\alpha) - \delta qdp(\sin^2\alpha + \cos^2\alpha) \\
&= \delta pdq - \delta qdp
\end{aligned}
$$

Hence

$$P\,dQ - \delta Q\,dP = \delta pdq - \delta qdp$$

Thus bilinear form remains invariant i.e.

and transformation (q_j, p_j) set to (Q_j, P_j) set is canonical .

Alternative

An Exact Differentiation condition

We have to prove

$$\sum_j p_j dq_j - \sum_j P_j dQ_j = dF$$

i.e. $pdq - PdQ = pdq - (q\sin\alpha + p\cos\alpha)d(q\cos\alpha - p\sin\alpha)$

$$
\begin{aligned}
&= pdq - (q\sin\alpha + p\cos\alpha)(dq\cos\alpha - dp\sin\alpha) \\
&= pdq - (q\sin\alpha.dq\cos\alpha - q\sin\alpha.dp\sin\alpha) \\
&\quad -(p\cos\alpha.dq\cos\alpha - p\cos\alpha.dp\sin\alpha)
\end{aligned}
$$

$$= pdq - \left(qdq \sin\alpha \cos\alpha - qdp \sin^2\alpha \right)$$
$$- \left(pdq \cos^2\alpha - pdp \sin\alpha \cos\alpha \right)$$
$$= pdq \left(1 - \cos^2\alpha \right) - \left(qdq \sin\alpha \cos\alpha - qdp \sin^2\alpha \right)$$
$$+ \left(pdp \sin\alpha \cos\alpha \right)$$
$$= pdq \sin^2\alpha + qdp \sin^2\alpha$$
$$- \left(qdq \sin\alpha \cos\alpha + pdp \sin\alpha \cos\alpha \right)$$
$$= pdq \sin^2\alpha + qdp \sin^2\alpha \quad - \left(qdq \sin\alpha \cos\alpha + pdp \sin\alpha \cos\alpha \right)$$
$$= pdq \sin^2\alpha + qdp \sin^2\alpha \quad - \left(qdq \sin\alpha \cos\alpha + pdp \sin\alpha \cos\alpha \right)$$
$$= \left(pdq + qdp \right) \sin^2\alpha \quad - \left(qdq + pdp \right) \left(\sin\alpha \cos\alpha \right)$$
$$= d(pq) \sin^2\alpha \quad - d\left(\frac{q^2 + p^2}{2} \right) \left(\sin\alpha \cos\alpha \right)$$
$$= d\left[pq \sin^2\alpha + \left(\frac{q^2 + p^2}{2} \right) \left(\sin\alpha \cos\alpha \right) \right]$$
$$= dF$$

i.e. $pdq - PdQ$ is an exact differential, then transformation is canonical.

Where $F = pq \sin^2\alpha + \left(\frac{q^2 + p^2}{2} \right) \left(\sin\alpha \cos\alpha \right)$

Example 2: Show that the transformation defined by

$$q = \sqrt{2P} \sin\theta$$
$$p = \sqrt{2P} \cos\theta$$

is canonical

Sol. We shall use the Poisson bracket condition.

$$[Q, Q]_{p,q} = [P, P]_{p,q} = 0 \qquad \text{and} \qquad [P, Q]_{p,q} = 1$$

The above transformation (1) can be written as

$$\tan Q = \frac{q}{p}$$

$$P = \frac{1}{2}(q^2 + p^2)$$

Therefore the P.B. $[P, Q]_{p,q}$ can be written as

$$[P, Q]_{p,q} = \frac{\partial P}{\partial p}\frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q}\frac{\partial Q}{\partial p}$$

$$\frac{\partial P}{\partial p} = \frac{1}{2} \times 2p = p$$

$$\frac{\partial P}{\partial q} = \frac{1}{2} \times 2q = q$$

$$\frac{\partial Q}{\partial q} = \frac{1}{\sec^2 Q} \cdot \frac{1}{p} = \frac{\cos^2 Q}{p}$$

$$\frac{\partial Q}{\partial p} = \frac{1}{\sec^2 Q} \cdot \left(\frac{-q}{p^2}\right) = -\cos^2 Q \frac{q}{p^2}$$

Substituting in the P.B. $[Q, P]$ we find

$$[P, Q]_{p,q} = \frac{\partial P}{\partial p} \cdot \frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q} \cdot \frac{\partial Q}{\partial p}$$

$$= p \cdot \frac{\cos^2 Q}{p} - q(-\cos^2 Q)\frac{q}{p^2}$$

$$= \cos^2 Q \left\{1 + \frac{q^2}{p^2}\right\}$$

$$= \cos^2 Q \left\{1 + \tan^2 Q\right\}$$

$$= \cos^2 Q \times \sec^2 Q = 1$$

Hence the given transformation is canonical.

Example 3: Show that the transformation

$$Q = \sqrt{2q}e^{\alpha} \cos p$$
$$P = \sqrt{2q}e^{-\alpha} \sin p$$

is a canonical transformation.

Sol. We have to prove that the P.B. $[Q, P]_{q,p}$ is equal to 1.

$$[\mathrm{Q},\mathrm{P}]_{q,p} = \frac{\partial Q}{\partial q}.\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}.\frac{\partial P}{\partial q}$$

$$= \frac{\partial}{\partial q}\left(\sqrt{2q}e^{\alpha}\cos p\right).\frac{\partial}{\partial p}\left(\sqrt{2q}e^{-\alpha}\sin p\right)$$

$$-\frac{\partial}{\partial p}\left(\sqrt{2q}e^{\alpha}\cos p\right).\frac{\partial}{\partial q}\left(\sqrt{2q}e^{-\alpha}\sin p\right)$$

$$= \left(\sqrt{2}\frac{1}{2\sqrt{q}}e^{\alpha}\cos p\right).\left(\sqrt{2q}e^{-\alpha}\cos p\right)$$

$$-\left(-\sqrt{2q}e^{\alpha}\sin p\right).\left(\sqrt{2}\frac{1}{2\sqrt{q}}e^{-\alpha}\sin p\right)$$

$$= \left(\frac{1}{\sqrt{q}}e^{\alpha}\cos p\right).\left(\sqrt{q}e^{-\alpha}\cos p\right)$$

$$+\left(\sqrt{q}e^{\alpha}\sin p\right).\left(\frac{1}{\sqrt{q}}e^{-\alpha}\sin p\right)$$

$$= \cos^2 p + \sin^2 p = 1$$

Alternative

An Exact Differentiation condition

We have to prove

$$\sum_j p_j dq_j - \sum_j P_j dQ_j = dF$$

i.e. $pdq - PdQ$

$$= pdq - \sqrt{2q}e^{-\alpha}\sin p\; d\left(\sqrt{2q}e^{\alpha}\cos p\right)$$

$$= pdq - \sqrt{2q}e^{-\alpha}\sin p\left\{\frac{1}{2\sqrt{q}}\sqrt{2}e^{\alpha}\cos p dq + \sqrt{2q}e^{\alpha}\left(-\sin p\right)dpd\right\}$$

$$= pdq - \left\{\sqrt{2q}e^{-\alpha}\sin p\frac{1}{2\sqrt{q}}\sqrt{2}e^{\alpha}\cos p dq\right.$$

$$\left.-\sqrt{2q}e^{-\alpha}\sin p\sqrt{2q}e^{\alpha}\sin p dp\right\}$$

$$= pdq - \sin p \cos p dq + 2q \sin^2 p dp$$

$$= \left(p - \sin p \cos p\right) dq + 2q \sin^2 p dp \qquad (1)$$

$$= \left(p - \frac{1}{2}\sin 2p\right) dq + q(1 - \cos 2p) dp$$

$$= \left(p - \frac{1}{2}\sin 2p\right) dq + qd\left(p - \frac{1}{2}\sin 2p\right)$$

$$= \left(p - \frac{1}{2}\sin 2p\right) dq + qd\left(p - \frac{1}{2}\sin 2p\right)$$

$$= d\left\{\left(p - \frac{1}{2}\sin 2p\right) q\right\}$$

$$= dF$$

$pdq - PdQ$ is an exact differential, then transformation is canonical.

where $F = \left(p - \frac{1}{2}\sin 2p\right) q$

We can prove exact differential condition directly as given below

We can write from eq.(1)

$$\left(p - \sin p \cos p\right) dq + 2q \sin^2 p dp = Mdq + Ndp$$

where $\left(p - \sin p \cos p\right) = M$

$$2q \sin^2 p = N$$

Exact differential condition is given by

$$\frac{\partial M}{\partial p} = \frac{\partial N}{\partial q}$$

Applying this condition here

$$\text{L.HS.} = \frac{\partial M}{\partial p} = \frac{\partial}{\partial p}\left(p - \sin p \cos p\right)$$

$$= \frac{\partial}{\partial p}\left(p - \frac{1}{2}\sin 2p\right)$$

$$= 1 - \cos 2p = 2\sin^2 p$$

$$\text{RHS} = \frac{\partial N}{\partial q} = \frac{\partial}{\partial q}\left(2q\sin^2 p\right)$$

$$= 2\sin^2 p$$

Hence LHS=RHS and eq.(i) is in exact differential form and transformation is canonical

Alternative

Bilinear Invariant Condition

Here $\sum_j \left(\delta P_j dQ_j - \delta Q_j dP_j\right)$

$$= \delta P\, dQ - \delta Q\, dP$$

$$= \delta\left(\sqrt{2q}e^{-\alpha}\sin p\right) d\left(\sqrt{2q}e^{\alpha}\cos p\right) - \delta\left(\sqrt{2q}e^{\alpha}\cos p\right) d\left(\sqrt{2q}e^{-\alpha}\sin p\right)$$

$$= \delta\left(\sqrt{2q}e^{-\alpha}\sin p\right) d\left(\sqrt{2q}e^{\alpha}\cos p\right) - \delta\left(\sqrt{2q}e^{\alpha}\cos p\right) d\left(\sqrt{2q}e^{-\alpha}\sin p\right)$$

$$= 2\delta\left(\sqrt{q}\sin p\right) d\left(\sqrt{q}\cos p\right) - 2\delta\left(\sqrt{q}\cos p\right) d\left(\sqrt{q}\sin p\right)$$

$$= 2\left(\frac{1}{2\sqrt{q}}\sin p\delta q + \sqrt{q}\cos p\delta p\right)\left(\frac{1}{2\sqrt{q}}\cos pdq - \sqrt{q}\sin pdp\right)$$

$$-2\left(\frac{1}{2\sqrt{q}}\cos p\delta q - \sqrt{q}\sin p\delta p\right)\left(\frac{1}{2\sqrt{q}}\sin pdq + \sqrt{q}\cos pdp\right)$$

$$= \left(\frac{1}{2q}\sin p\cos p\delta q\, dq + \cos^2 p\,\delta p dq - \sin^2 p\delta q dp - 2q\cos p\sin p\delta p dp\right)$$

$$-\left(\frac{1}{2q}\sin p\cos p\delta q\, dq + \cos^2 p\,\delta q dp - \sin^2 p\delta p dq - 2q\cos p\sin p\delta p dp\right)$$

$$= \left(\cos^2 p\,\delta p dq - \sin^2 p\delta q dp\right) - \left(\cos^2 p\,\delta q dp - \sin^2 p\delta p dq\right)$$

$$= \left(\cos^2 p + \sin^2 p\right)\delta p dq - \left(\cos^2 p + \sin^2 p\right)\delta q dp$$

$$= (1)\delta p dq - (1)\delta q dp$$

$$= \delta p dq - \delta q dp$$

Hence

$$P\,dQ - \delta Q\,dP = \delta\, pdq - \delta qdp$$

Thus bilinear form remains invariant i.e.

and transformation $(q_{j,}p_j)$ set to $(Q_{j,}P_j)$ set is canonical .

9.7 Self Learning Exercise

Q.1 Show that $ad - bc = 1$ is order that the transformation.

$$Q = aq + bp$$
$$P = cq + d\,p \text{ is canonical.}$$

Q.2 Deduce the relations for $S = S(\vec{r}, t)$

$$\vec{P} = \nabla S\,,\; H = -\frac{\partial S}{\partial t}$$

9.8 Illustrative Examples

Example 4: Show that the transformation

$$Q = \frac{1}{p},\; P = qp^2 \text{ is canonical}$$

Sol. $$[\mathrm{Q,P}]_{q,p} = \frac{\partial Q}{\partial q}.\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}$$

$$= \frac{\partial}{\partial q}\left(\frac{1}{p}\right).\frac{\partial}{\partial p}\left(qp^2\right) - \frac{\partial}{\partial p}\left(\frac{1}{p}\right)\frac{\partial}{\partial q}\left(qp^2\right)$$

$$= 0.\left(2qp\right) - \left(-\frac{1}{p^2}\right)\left(p^2\right)$$

$$= 1$$

Hence transformation is canonical.

Alternative

An Exact Differentiation condition

We have to prove

$$\sum_j p_j dq_j - \sum_j P_j dQ_j = dF$$

i.e. $pdq - PdQ$

$$= pdq - qp^2 d\left(\frac{1}{p}\right)$$

$$= pdq - qp^2\left(-\frac{1}{p^2}dp\right)$$

$$= pdq + qdp$$

$$= d(pq)$$

$$= dF$$

$pdq - PdQ$ is an exact differential, then transformation is canonical.

where $F = pq$

Alternative

Bilinear Invariant Condition

Here $\sum_j \left(\delta P_j dQ_j - \delta Q_j dP_j\right)$

$$= \delta P\, dQ - \delta Q\, dP$$

$$= \delta(qp^2)\, d\left(\frac{1}{p}\right) - \delta\left(\frac{1}{p}\right) d(qp^2)$$

$$= (\delta qp^2 + 2qp\delta p)\left(-\frac{1}{p^2}dp\right) - \left(-\frac{1}{p^2}\delta p\right)(dqp^2 + 2qpdp)$$

$$= \delta qp^2\left(-\frac{1}{p^2}dp\right) + 2qp\delta p\left(-\frac{1}{p^2}dp\right)$$

$$+ dqp^2\left(\frac{1}{p^2}\delta p\right) + 2qpdp\left(\frac{1}{p^2}\delta p\right)$$

$$= -\delta q dp - 2q\frac{1}{p}\delta p dp + dq\delta p + 2q\frac{1}{p}dp\delta p$$

$$= dq\delta p - \delta q dp$$

Hence

$$P\, dQ - \delta Q\, dP = \delta p dq - \delta q dp$$

Thus bilinear form remains invariant i.e. and transformation (q_j, p_j) set to (Q_j, P_j)

set is canonical .

Example 5: Show that the transformation

$$P = q\cot p$$

$$Q = \log\left(\frac{\sin p}{q}\right) \text{is canonical.}$$

and show that the generating function is

$$F = e^{-Q}\left(1 - q^2 e^{2Q}\right)^{\frac{1}{2}} = q\sin^{-1}\left(qe^{Q}\right)$$

Sol. We have to prove that the P.B. $[\mathrm{Q},\mathrm{P}]_{q,p}$ is equal to 1.

$$[\mathrm{Q},\mathrm{P}]_{q,p} = \frac{\partial Q}{\partial q}.\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}.\frac{\partial P}{\partial q}$$

$$= \frac{\partial}{\partial q}\left(\log\left(\frac{1}{q}\sin p\right)\right).\frac{\partial}{\partial p}(q\cot p) - \frac{\partial}{\partial p}\left(\log\left(\frac{1}{q}\sin p\right)\right).\frac{\partial}{\partial q}(q\cot p)$$

$$= \frac{1}{\left(\frac{1}{q}\sin p\right)}\frac{-1}{q^2}\sin p.\left(-q\cos ec^2 p\right) \quad - \frac{1}{\left(\frac{1}{q}\sin p\right)}\frac{1}{q}\cos p.\left(\cot p\right)$$

$$= \cos ec^2 p - \cot^2 p$$

$$= 1$$

We shall show that if F is the generating function of the given canonical transformation, then

$$dF = pdq + PdQ$$

$$\text{Now } dQ = \frac{\partial Q}{\partial q}dq + \frac{\partial Q}{\partial p}dp = -\frac{dq}{q} + \cot p dp$$

Therefore if $F(q,p)$ is generating function of canonical transformation

$$\mathrm{dF} = \mathrm{pdq} - P\,\mathrm{dQ} = \mathrm{pdq} - (\mathrm{qcotp})\left(-\frac{dq}{q} + \cot p dp\right)$$

$$= (p + \cot p)dq - q\cot^2 p dp$$

$$= \frac{\partial}{\partial q}(qp + q\cot p)dq + \frac{\partial}{\partial p}[\mathrm{qp} + \mathrm{qcotp}]\mathrm{dp}$$

or $dF = \frac{\partial F}{\partial q} dq + = \frac{\partial F}{\partial p} dp$

which shows that the right hand side is the exact differential of the function

$$F = qp + qcotp$$

To obtain the given form, let us put

$$Q = \log\left(\frac{sinp}{q}\right)$$

$$\text{or } \sin p = qe^{Q}$$

$$\cos p = \left(1 - q^2 e^{2Q}\right)^{\frac{1}{2}}$$

$$\cot p = \frac{\left(1 - q^2 e^{2Q}\right)^{\frac{1}{2}}}{qe^{Q}}$$

Putting these values in the expression for F, we get

$$F = q\sin^{-1}(\mathrm{qe}^{Q}) + \mathrm{e}^{-Q}(1 - \mathrm{q}^2\mathrm{e}^{2Q})^{\frac{1}{2}}$$

$$F = -\left(e^{Q} - 1\right)^2 \tan p$$

Example 6 : Using Poisson bracket, show that the transformation

$$Q = \left(e^{-2q} - p^2\right)^{1/2}, \qquad P = \cos^{-1}\left(pe^{q}\right) \quad \text{is canonical.}$$

Sol. We have the derivatives

$$\frac{\partial Q}{\partial q} = \frac{-e^{-2q}}{\left(e^{-2q} - p^2\right)^{1/2}}, \qquad \frac{\partial Q}{\partial p} = \frac{-p}{\left(e^{-2q} - p^2\right)^{1/2}}$$

$$\frac{\partial P}{\partial q} = \frac{-p}{\left(e^{-2q} - p^2\right)^{1/2}}, \qquad \frac{\partial P}{\partial p} = \frac{-1}{\left(e^{-2q} - p^2\right)^{1/2}}$$

We have

$$[Q, P] = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q}$$

$$= \left(\frac{-e^{-2q}}{\left(e^{-2q} - p^2\right)^{1/2}} \right) \left(\frac{-1}{\left(e^{-2q} - p^2\right)^{1/2}} \right) - \left(\frac{-p}{\left(e^{-2q} - p^2\right)^{1/2}} \right) \left(\frac{-p}{\left(e^{-2q} - p^2\right)^{1/2}} \right)$$

$$= \left(\frac{-e^{-2q}}{\left(e^{-2q} - p^2\right)} \right) - \left(\frac{p^2}{\left(e^{-2q} - p^2\right)} \right) = 1$$

9.9 Summary

We have introduced action S(q, t) as a function of coordinate and time. We derive the differential of action S as $dS = \sum_i p_i \, dq_i - H \, dt$ and we find the important relations viz. $\frac{\partial S}{\partial q_i} = p_i$ and $\frac{\partial S}{\partial t} = -H$. We derive generating functions for canonical transformation. We discuss the invariance of Poisson's brackets under canonical transformation.

9.10 Glossary

***Transformation*:** A process by which one figure, expression or function is converted into another one of similar value

9.11 Answers to Self Learning Exercise

Ans.1: We have to prove

$$[Q, P]_{q,p} = 1$$

L.H.S. $[Q, P]_{q,p} = \frac{\partial Q}{\partial q} . \frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p} . \frac{\partial P}{\partial q}$

$$= \frac{\partial}{\partial q}(aq + bp) . \frac{\partial}{\partial p}(cq + d\ p) - \frac{\partial}{\partial p}(aq + bp) . \frac{\partial}{\partial q}(cq + d\ p)$$

$$= (a.1 + 0).(0 + d.1) - (0 + b.1).(c.1 + 0)$$

$$= ad - bc$$

Therefore the given transformation will be canonical if $ad - bc = 1$.

9.12 Exercise

Q.1 If p and q are the position and momentum variables which one of the following is NOT a canonical transformation?

(A) $Q = \alpha q$ and $P = \frac{1}{\alpha} p$, for $\alpha \neq 0$

(B) $Q = \alpha q + \beta p$ and $P = \beta q + \alpha p$ for α, β real and $\alpha^2 - \beta^2 = 1$

(C) $Q = p, P = q$

(D) $Q = p, P = -q$

Q.2 The Lagrangian for a simple pendulum is given by

$$L = \frac{1}{2} ml^2 \dot{\theta}^2 - mgl(1 - \cos\theta)$$

Which of the following represents Hamilton's equations

(A) $\dot{p}_\theta = -mgl \sin\theta \; ; \; \dot{\theta} = \frac{p_\theta}{ml^2}$ (B) $\dot{p}_\theta = mgl \sin\theta \; ; \; \dot{\theta} = \frac{p_\theta}{ml^2}$

(C) $\dot{p}_\theta = m\ddot{\theta} \; ; \; \dot{\theta} = \frac{p_\theta}{m}$ (D) $\dot{p}_\theta = -\frac{g}{l}\theta \; ; \; \dot{\theta} = \frac{p_\theta}{ml}$

Q.3 Show that the transformation $Q_i = \alpha q_i, P_i = \beta p_i, \alpha \neq 0, \beta \neq 0$ is canonical and new Hamiltonian is $K = \alpha\beta H$ Where H is old Hamiltonian $H = H(q_i, p_i)$

Q.4 Obtain Hamilton's canonical equation from the principle of least action.

Q.5 Prove that the transformation

$q = \sqrt{2P}\sin Q$

$p = \sqrt{2P}\cos Q$ is canonical.

i.e. $P = \frac{1}{2}\left(p^2 + q^2\right)$ $, Q = \tan^{-1}\left(\frac{q}{p}\right)$ is canonical

Q.6 The transformation equations between two sets of coordinates are

$Q = \log(1 + q^{\frac{1}{2}}\cos p)$

$P = 2(1 + q^{\frac{1}{2}}\cos p)q^{\frac{1}{2}} \sin p$

(i) Show directly from these transformation equations that Q,P are canonical variables if q and p are.

(ii) Show that the function that generates this transformation is

$$F = -\left(e^{Q} - 1\right)^2 \tan p$$

9.13 Answers to Exercise

Ans.3: $[\mathrm{P}_i, \mathrm{Q}_i]_{p_i q_i} = 1$

$$\text{L.H.S.} = \frac{\partial P_i}{\partial q_i}.\frac{\partial Q_i}{\partial q_i} - \frac{\partial P_i}{\partial p_i}\frac{\partial Q_i}{\partial p_i}$$

$= \beta\alpha - 0$, thus the transformation will be canonical if $\beta\alpha = 1$. To prove that the given transformation is canonical, we write Hamilton's canonical equations for the variables q_i, p_i:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \Rightarrow \frac{\dot{Q}_i}{\alpha} = \beta\frac{\partial H}{\partial p_i}$$

$$\text{or } \dot{Q}_i = \frac{\partial(\alpha\beta\,\mathrm{H})}{\partial p_i} \equiv \frac{\partial H'}{\partial p_i}$$

Thus we find that Q_i and P_i satisfy the Hamilton's equations for the new Hamiltonian $H' = \alpha\beta\,\mathrm{H}$.

References and Suggested Readings

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UNIT–10
The Hamilton-Jacobi Equation

Structure of the Unit

10.0 Objectives

10.1 Introduction

10.2 The Hamilton-Jacobi equation

10.3 Complete integrals of the H-J equation by separation of variables

10.4 Application of the H-J method

10.5 Self Learning Exercise

10.6 Summary

10.7 Glossary

10.8 Answers to Self Learning Exercise

10.9 Exercise

10.10 Answers to Self Learning Exercise

References and Suggested Readings

10.0 Objectives

In this chapter we shall focus on the following topics of study

1. Hamilton-Jacobi equation
2. Complete integral of H-J equation
3. Solving H-J equation by the method of separation of variables
4. Cyclic coordinates
5. Solving Kepler's problem by H-J method
6. Solving simple harmonic oscillator problem by H-J method.

10.1 Introduction

The Canonical transformation leads us to the Hamilton-Jacobi theory which is an equivalent formulation of classical mechanics. Two slightly different approaches are available. In one, the procedure is to find a canonical

transformation from the original (q, p) to a new set of variables (Q, P) which makes all coordinates cyclic. Then the new momenta will be constant in time.The second approach is to effect a canonical transformation such that the new Hamiltonian is zero, then each $\dot{Q}_i$ and $\dot{P}_i$ is zero. It means that all Q's and P's will be constant of motion. The second approach is a more general one and we shall discuss such a transformation in this chapter.

10.2 The Hamilton-Jacobi Equation

The action $S(q,t)$ has been considered as a function of coordinates and time, and it has been shown that the partial derivative of $S(q,t)$ with respect to time is related to the Hamiltonian by

$$\boxed{\frac{\partial S}{\partial t} + H(q,p,t) = 0} \tag{1}$$

Replacing The momenta p in the Hamiltonian by the derivatives $\frac{\partial S}{\partial q}$, we have the equation

$$\frac{\partial S}{\partial t} + H\left(q_1,....q_s;\frac{\partial S}{\partial q_1},.....\frac{\partial S}{\partial q_s};t\right) = 0 \tag{2}$$

This first-order partial differential equation is known as Hamilton-Jacobi equation (H-J equation).

Like Lagrange's equations and canonical equations, the H-J equation is the basis of a general Method of integrating equations of motion

Method of integrating equations of motion

Before describing this method we should recall that every first order partial differential equation has a solution depending on an arbitrary function; such a solution is called the "general integral of the H-J equation".

In mechanical applications, the general integral of H-J equation is less important than a complete integral, which contains as many independent arbitrary constants as there are independent variables. In the H-J equation the independent variables are the time and $s+1$ coordinates i.e. $;\alpha_1,\alpha_2,.....\alpha_s$ *and* A are arbitrary constants.

Let us now ascertain the relation between a complete integral of the H-J equation and the solutions of the equations of motion which is of interest.

We write $S = f(t, q_1, ...q_s; \alpha_1, ...\alpha_s) + A$ where $\alpha_1, ...\alpha_s$ and A are arbitrary constants.

To do this we affect canonical transformation from *q, p* to new variables, taking the function $f(t, q, \alpha)$ as the generating function and the quantities $\alpha_1, \alpha_2, ...\alpha_s$ as the new momenta.

Let the new coordinates be $\beta_1, \beta_2, ...\beta_s$.

Since the generating function depends on the old coordinates and new momenta.

$$p_i = \frac{\partial f}{\partial q_i}, \beta_i = \frac{\partial f}{\partial \alpha_i}, H' = H + \frac{\partial f}{\partial t}. \tag{4}$$

But since the function *f* satisfies H-J equation, we see that the new Hamiltonian is zero.

$$H' = H + \frac{\partial f}{\partial t} = H + \frac{\partial S}{\partial t} = 0 \tag{5}$$

Hence the canonical equations in the new variables are

$$\dot{\alpha}_i = 0, \dot{\beta}_i = 0$$

Therefore α_i = constant

β_i = constant

So by means of *s* equations $\frac{\partial f}{\partial \alpha_i} = \beta_i$, the *s*-coordinates *q* can be expressed in terms of the time and the *2s* constants α and β.

This gives the general integral of the equations of motion.

Thus the solution of the problem of the motion of a mechanical system by H-J method proceeds as follows :

(1) From the Hamiltonian, we form the H-J equation and find its complete integral
$\{viz.\ S = f(t, q_1 .....q_s; \alpha_1 .....\alpha_s) + A\}$

(2) Differentiating this with respect to arbitrary constants α and equating the derivatives to new constants β, we obtain *s* algebraic equations.

$$\frac{\partial S}{\partial \alpha_i} = \beta_i$$

Whose solutions give the coordinates q as functions of time and $2s$ arbitrary constants.

The momenta as function of time may then be found from equations $p_i = \frac{\partial f}{\partial q_i}$.

The H-J equation takes a somewhat simpler form if the function H does not involve the time explicitly i.e. if the system is conservative.

As $\boxed{\frac{\partial S}{\partial t} = -H}$,

Therefore $\boxed{S = -\int H dt = -Et + S_0(\mathrm{q})}$ (6)

Where $S_0(q)$ is some function of coordinates only.

Substituting this value of S from (6) into H-J equation (2), the H-J equation takes the form :

$$\boxed{\frac{\partial S}{\partial t} + H\left(q; \frac{\partial S}{\partial q}; t\right) = 0} \qquad \text{(H-J equation)}$$

$$\text{Or } -E + H\left(q_1 \ldots\ldots q_s; \frac{\partial S_0}{\partial q_1} \ldots\ldots \frac{\partial S_0}{\partial q_s}\right) = 0$$

$$\text{or } H\left(q_1 \ldots\ldots q_s; \frac{\partial S_0}{\partial q_1} \ldots\ldots \frac{\partial S_0}{\partial q_s}\right) = E \qquad (7)$$

10.3 Complete Integrals of the H-J Equation by Separation of Variables

In a number of important cases, a complete integral of the H-J equation can be found by "separating the variables", a name given to the following method.

Let us assume that some coordinate, q_1 say and the corresponding derivatives $\frac{\partial S}{\partial q_1}$ appear in the H-J equation only in some combination $\phi\left(q_1, \frac{\partial S}{\partial q_1}\right)$ which does not involve the other coordinates, time, or derivatives, i.e. the equation is of the form

$$\Phi\left\{q_i, t, \frac{\partial S}{\partial q_i}, \frac{\partial S}{\partial t}, \phi\left(q_1, \frac{\partial S}{\partial q_1}\right)\right\} = 0 \tag{8}$$

where q_i denotes all the coordinates except q_1.

We seek a solution in the form of a sum

$$S = S'(\mathrm{q}_i, t) + \mathrm{S}_1(q_1) \tag{9}$$

Substituting (2) into (1) we get

$$\Phi\left\{q_i, t, \frac{\partial S'}{\partial q_i}, \frac{\partial S'}{\partial t}, \varphi\left(q_1, \frac{\partial S_1}{\partial q_1}\right)\right\} = 0 \tag{10}$$

Let us suppose that the solution (2) has been found. Then when it is substituted in (3), the latter must become an identity valid (in particular) for any value of the coordinate q_1.

When q_1, changes only the function ϕ is affected, and so, if (3) is an identity, ϕ must be a constant.

Thus equation (3) gives the two equations :

$$\phi\left(q_1, \frac{\partial S_1}{\partial q_1}\right) = \alpha_1 \qquad \alpha_1 \text{is an arbitrary constant.} \tag{11}$$

$$\Phi\left\{q_i, t, \frac{\partial S'}{\partial q_i}, \frac{\partial S'}{\partial t}, \alpha_1\right\} = 0 \tag{12}$$

The first of these is an ordinary differential equation and the function $\mathrm{S}_1(q_1)$ is obtained from it by simple integration.

The remaining partial differential equation involves fewer independent variables. If we can successively separate in this way all the *s* coordinates and the time, the finding of a complete integral of H-J equation is reduced to quadratures.

For a conservative system we have in practice to separate only *s* variables (the coordinates) and when this separation is complete the required integral is

$$S = \sum_k S_k(q_k; \alpha_1, \ldots\ldots \alpha_s) - \mathrm{E}(\alpha_1 \ldots\ldots \alpha_s)\,\mathrm{t} \tag{13}$$

where each of the function S_k depends on only one coordinate; the energy E, as a function of the arbitrary constants $\alpha_1 \ldots\ldots \alpha_s$, is obtained by substituting $S_0 = \sum_k S_k$ in (7).

A particular case is the separation of a cyclic variables. A cyclic coordinate does not appear explicitly in the Hamiltonian, nor therefore in the Hamilton-Jacobi

equation. Let q_1 be the cyclic coordinate.

The function $\phi\left(q_1, \frac{\partial S}{\partial q_1}\right)$ reduces to $\frac{\partial S}{\partial q_1}$ simply, as q_1 does not appear explicitly in the Hamiltonian.

Thus from eq. (4)

$$\frac{\partial S}{\partial q_1} = \alpha_1$$

Or integrating we get

$$S_1 = \alpha_1 q_1 + S'(q_i, t) \tag{14}$$

where q_i denotes all the coordinates except q_1.

The constant α_1 is just the constant value of the momentum $p_1 = \frac{\partial S}{\partial q_1}$ corresponding to the ***cyclic coordinate***.

The appearance of the time in the term *–Et* for a conservative system corresponds to the separation of the "Cyclic Variable" *t*.

It should be noted that the Hamilton-Jacobi treatment is the most powerful method of finding the general integral of the equations of motion. To make the variables separable in H-J equation, the coordinates must be appropriately chosen.

In the following we shall consider some examples of separating the variables in different coordinates, which may be of physical interest in connection with problems of the motion of a particle in various external fields.

Separation of variables in spherical coordinates :

In spherical coordinates the Hamiltonian of a particle can be written as

$$\boxed{H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta}\right) + U(r, \theta, \phi)} \tag{1}$$

and the variables can be separated if

$$U = a(r) + \frac{b(\theta)}{r^2} + \frac{c(\phi)}{r^2 \sin^2\theta}, \qquad \text{where} \quad a(r), b(\theta), C(\phi) \text{ are arbitrary}$$

functions,

The last term in this expression for U is unlikely to be of physical interest, and we shall therefore take

$$U = a(r) + \frac{b(\theta)}{r^2} \tag{2}$$

If H does not depend explicitly on *t*, we can express $S = S_0(q) - Et$.

In this the Hamilton-Jacobi equation for the function S_0 is

$$H\left(q_1,.....q_s;\frac{\partial S_0}{\partial q_1},.....,\frac{\partial S_0}{\partial q_s}\right) = E \tag{3}$$

Making use of the Hamiltonian (1) and replacing

$p_r = \frac{\partial S_0}{\partial r}, p_\theta = \frac{\partial S_0}{\partial \theta}, p_\phi = \frac{\partial S_0}{\partial \phi}$, we get the following equation.

$$\frac{1}{2m}\left(\frac{\partial S_0}{\partial r}\right)^2 + a(r) + \frac{1}{2mr^2}\left(\left(\frac{\partial S_0}{\partial \theta}\right)^2 + 2mb(\theta)\right) + \frac{1}{2mr^2\sin^2\theta}\left(\frac{\partial S_0}{\partial \phi}\right)^2 = E \tag{4}$$

In the above equation (4), ϕ does not appear explicitly, so the coordinate ϕ is cyclic.

We seek a solution in the form

$$S_0 = p_\phi \phi + S_1(r) + S_2(\theta),$$

obtaining for the functions $S_1(r)$ and $S_2(\theta)$ the equations

$$\frac{1}{2m}\left(\frac{dS_1}{dr}\right)^2 + a(r) + \frac{1}{2mr^2}\left(\left(\frac{dS_2}{d\theta}\right)^2 + 2mb(\theta)\right) + \frac{p_\phi^2}{2mr^2\sin^2\theta} = E$$

$$\text{Or } \frac{1}{2m}\left(\frac{dS_1}{dr}\right)^2 + a(r) + \frac{1}{2mr^2}\left(\left(\frac{dS_2}{d\theta}\right)^2 + 2mb(\theta) + \frac{p_\phi^2}{\sin^2\theta}\right) = E \tag{5}$$

$$\text{Let } \left(\frac{dS_2}{dr}\right)^2 + 2mb(\theta) + \frac{p_\phi^2}{\sin^2\theta} = \beta \tag{6}$$

The equation (5) can be written as

$$\frac{1}{2m}\left(\frac{dS_1}{dr}\right)^2 + a(r) + \frac{\beta}{2mr^2} = E \tag{7}$$

Integration gives

$$S = -Et + p_\phi\phi + \int\sqrt{\left\{\beta - 2mb(\theta) - \frac{p_\phi^2}{\sin^2\theta}\right\}}\,d\theta + \int\left[2m\{E - a(r)\} - \frac{\beta}{r^2}\right]^{\frac{1}{2}} dr$$

where p_ϕ, β, E are arbitrary constants; on differentiating with respect to these and equating the results to other constants, we have the general solution of the equations of motion.

10.4 Application of the H-J Method

(A) Kepler's problem:

In the Kepler's problem the potential energy of a particle is

$$U = -\frac{k}{r} \qquad (k \text{ is constant}) \tag{1}$$

The Hamiltonian of the particle is

$$\boxed{H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) + \left(-\frac{k}{r}\right)} \tag{2}$$

$\frac{\partial S}{\partial t} = -H = -E$, (Where energy E is constant)

Therefore $S = -Et + S_0(q)$

Hamilton-Jacobi equation is

$$-E + H\left(q_1, ...q_s; \frac{\partial s_0}{\partial q_1} ..... \frac{\partial s_0}{\partial q_s}\right) = 0$$

For the Hamiltonian (2), this equation is

$$\frac{1}{2m}\left(\frac{\partial s_0}{\partial r}\right)^2 + \frac{1}{2mr^2}\left(\frac{\partial s_0}{\partial \theta}\right)^2 - \frac{k}{r} = E$$

$$\text{or } \frac{1}{2m}\left(\frac{\partial S_0}{\partial r}\right)^2 + \frac{1}{2mr^2}\left(\frac{\partial S_0}{\partial \theta}\right)^2 - \frac{k}{r} = E \tag{3}$$

As the ***coordinate θ is cyclic, so p_θ is conserved.***

We express $S_0 = p_\theta \theta + S_1(r)$ So the equation (3) becomes

$$\frac{1}{2m}\left(\frac{dS_1}{dr}\right)^2 - \frac{k}{r} + \frac{1}{2mr^2} p_\theta^2 = E$$

Solving, we find

$$\left(\frac{dS_1}{dr}\right)^2 = 2m\left[E + \frac{k}{r} - \frac{p_\theta^2}{2mr^2}\right]$$

$$\text{or } S_1 = \int \sqrt{2m\left[E + \frac{k}{r} - \frac{p_\theta^2}{2mr^2}\right]}\, dr$$

So the solution is

$$S = p_\theta \theta + \int \sqrt{2m\left[E + \frac{k}{r} - \frac{p_\theta^2}{2mr^2}\right]}\, dr - Et \tag{4}$$

$$= f(\mathrm{q}_1, \ldots \mathrm{q}_s; \ldots\ldots \alpha_1, \ldots\ldots \alpha_s) + \mathrm{A}$$

Using he equations

$$\frac{\partial f}{\partial \alpha_i} = \beta_i \quad \text{Gives} \quad \frac{\partial S}{\partial E} = \beta_1$$

(here we are differentiating w.r.t. E which is the variable α_1)

$$\text{or } \beta_1 = -t + \frac{\partial S_0}{\partial E}$$

$$\text{or } t + \beta_1 = \int \frac{1}{2} \frac{\sqrt{2m}}{\sqrt{2m\left(E + \frac{k}{r} - \frac{p_\theta^2}{2mr^2}\right)}} dr$$

Similarly

$$\beta_2 = \frac{\partial f}{\partial \alpha_2} \qquad (\alpha_2 = p_\theta)$$

$$\theta = \beta_2 = \int \frac{p_\theta dr}{r^2 \sqrt{2m\left(E + \frac{k}{r}\right) - \frac{p_\theta^2}{r^2}}}$$

Integrating the above equation, we find

$$\frac{p_\theta^2}{mkr} = 1 + \frac{p_\theta}{mk}\left(2mE + \frac{mk^2}{p_\theta^2}\right)^{\frac{1}{2}} \cos(\theta - \beta_2)$$

$$\text{or } \boxed{\frac{p}{r} = 1 + e\cos\psi}$$

(equation of the conic-section)

$$\text{where } P = \frac{p_\theta^2}{mk} \text{ and eccentricity } e = \left(1 + \frac{2Ep_\theta^2}{mk^2}\right)^{\frac{1}{2}}$$

The equation of the trajectory of the particle is conic section with one focus at the origin.

(B) Harmonic oscillator problem as an example of H-J method :

The Hamiltonian is

$$H = \frac{1}{2m}(\mathrm{p}^2 + \mathrm{m}^2\,\omega^2\,\mathrm{q}^2) \equiv \mathrm{E},$$

The Hamilton-Jacobi equation is

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial q}\right)^2 + m^2\omega^2 q^2\right] + \frac{\partial S}{\partial t} = 0$$

We express $S(q,t) = S_0(q) - \mathrm{Et}$

$$\frac{1}{2m}\left[\left(\frac{\partial S_0}{\partial q}\right)^2 + m^2\omega^2 q^2\right] = E$$

Integrating, we find

$$S_0 = \int \sqrt{\left(2mE - \frac{1}{2}m\omega^2 q^2\right)}dq$$

Therefore

$$S = \int \sqrt{\left(2mE - \frac{1}{2}m\omega^2 q^2\right)}dq - Et$$

$$\beta = \frac{\partial S}{\partial E} = \int \frac{1}{2}\frac{2m\ dq}{\left[2mE - \frac{1}{2}m\omega^2 q^2\right]^{\frac{1}{2}}} - t$$

Integrating and rearranging we find

$$q = \frac{2\sqrt{E}}{\omega}\sin\left(\frac{\omega t}{\sqrt{2m}} + \frac{\omega\beta}{\sqrt{2m}}\right)$$

Example 10.1 Solve the Hamilton-Jacobi equation for the given system for which Hamiltonian is given by

$$H = \frac{p^2}{2} - \frac{\beta}{q}$$

Sol. H.J. Equation is

$$\frac{1}{2}\left(\frac{\partial s}{\partial q}\right)^2 - \frac{\beta}{q} + \frac{\partial s}{\partial t} = 0$$

Let solution be

$$s = f(t) + \phi(q)$$

Using above equations ,we get

$$\frac{\partial f}{\partial t} + \frac{1}{2}\left(\frac{\partial \phi}{\partial q}\right)^2 - \frac{\beta}{q} = 0$$

which can be satisfied by writing

$$\frac{\partial f}{\partial t} = \frac{\beta}{q} - \frac{1}{2}\left(\frac{\partial \phi}{\partial q}\right)^2$$

$$= \frac{\mu}{\alpha} \qquad \text{Here } \alpha \text{ is a constant.}$$

From

$$\frac{\partial f}{\partial t} = \frac{\beta}{\alpha}$$

$$f = \frac{\beta}{\alpha} t$$

and $$\frac{\beta}{q} - \frac{1}{2}\left(\frac{\partial \phi}{\partial q}\right)^2 = \frac{\beta}{\alpha}$$

After integration

$$\phi(q) = \sqrt{2\beta\alpha}\sin^{-1}\sqrt{\frac{q}{\alpha}} + \left[\frac{2\beta q(\alpha - q)}{\alpha}\right]^{\frac{1}{2}}$$

Example 10.2 Solve the problem of a projectile which is projected with speed v_0 at an angle α with the horizontal by using Hamilton Jacobi method.

Sol. Hamiltonian is given by

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + mgy = E\,.$$

We consider the following Hamilton's characteristic function

$$W = W_x + W_y$$

We have $$H = \frac{1}{2m}\left[\left(\frac{\partial W_x}{\partial x}\right)^2 + \left(\frac{\partial W_y}{\partial y}\right)^2\right] + mgy = E\,,$$

Since

$$p_x = \left(\frac{\partial W_x}{\partial x}\right) \text{ and } p_y = \left(\frac{\partial W_y}{\partial y}\right)$$

So,

$$\left(\frac{\partial W_x}{\partial x}\right)^2 + \left(\frac{\partial W_y}{\partial y}\right)^2 = 2m\left(E - mgy\right)$$

$$W_y = \int \left[2m(E - mgy) - p_x^2 \right]^{\frac{1}{2}} dy$$

So $W = W_x + W_y$

$$W = p_x x + \int \left[2m(E - mgy) - p_x^2 \right]^{\frac{1}{2}} dy$$

Hamilton's principal function S is

$$S = W - Et$$

Here $H = -\frac{\partial S}{\partial t} = \alpha = E$

Thus We have

$$S = p_x x + \int \left[2m(E - mgy) - p_x^2 \right]^{\frac{1}{2}} dy - Et \qquad (1)$$

and $\beta = \frac{\partial S}{\partial \alpha} = \frac{\partial S}{\partial E}$

$$= m \int \frac{dy}{\sqrt{\left[2m(E - mgy) - p_x^2 \right]}} - t$$

or $$(\beta + t) = m \int \frac{dy}{\sqrt{\left[2m(E - mgy) - p_x^2 \right]}} - t \qquad (2)$$

By generating function W, we can write

$$\beta_x = \frac{\partial W}{\partial p_x}$$

$$= x - \int \frac{p_x dy}{\left[2m(E - mgy) - p_x^2 \right]^{1/2}}$$

$$= x + \frac{p_x}{m^2 g} \left[2mE - 2m^2 gy - p_x^2 \right]^{1/2}$$

If we put $\beta_x = x_0$,

(since β_x is constant)

Then we have $(x - x_0) = -\frac{p_x}{m^2 g} \left[2mE - p_x^2 - 2m^2 gy \right]^{1/2}$

or $$(x-x_0)^2 = \frac{p_x^2}{m^4 g^2} - \left[2mE - p_x^2 - 2m^2 gy\right]$$

$$= \frac{2p_x^2}{m^2 g}\left[\frac{2mE - p_x^2}{2m^2 g} - y\right]$$

or $$\frac{1}{2}\frac{m^2 g(x-x_0)^2}{p_x^2} = \left(\frac{2mE - p_x^2}{2m^2 g}\right) - y \qquad (3)$$

We assume the constant term

$$\frac{2mE - p_x^2}{2m^2 g} = y_0$$

From eq. (3)

$$y = y_0 - \frac{1}{2}\frac{m^2 g(x-x_0)^2}{p_x^2}$$

But we have $p_x = m\dot{x}$ (4)

$$= mv_0 \cos\alpha$$

So that $y = y_0 - \frac{1}{2}\frac{m^2 g(x-x_0)^2}{v_0^2 \cos^2\alpha}$ (5)

which is the equation of a parabola. Thus path of projectile is a parabola.

On solving eq. (2), we get

$y = y_0 - \frac{1}{2}g(t+\beta)^2$ which with $\beta = -t_0$ becomes

$$y = y_0 - \frac{1}{2}g(t-t_0)^2 \qquad (6)$$

From eq. (4),

$$m\dot{x} = p_x$$

or $$\int_{x_0}^{x} dx = \int_{t_0}^{t} \frac{p_x}{m} dt$$

or $$x = x_0 + \frac{p_x}{m}(t-t_0) \qquad (7)$$

Eqs. (5), (6), (7), describe the motion of the projectile.

10.5 Self Learning Exercise

Q.1 Write down the Hamilton-Jacobi equation.

Q.2 Apply Hamilton-Jacobi equation to the problem of one-dimensional harmonic oscillator.

Example 10.3 By using Hamilton Jacobi method, solve the problem of particle falling freely.

Sol. Let Hamiltonian of the system is

$$H = T + V(q)$$

$$= \frac{p^2}{2m} + mgy = E(total\,energy) \tag{1}$$

where we take y axis in the vertical direction (here q is y)

Using $p = \frac{\partial S}{\partial y}$, the Hamiltonian becomes

$$H(y, p, t) = \frac{1}{2m}\left(\frac{\partial S}{\partial y}\right)^2 + mgy \tag{2}$$

For the new Hamiltonian K to be zero , we have

$$H + \frac{\partial S}{\partial t} = 0$$

$$\frac{1}{2m}\left(\frac{\partial S}{\partial y}\right)^2 + mgy + \frac{\partial S}{\partial t} = 0 \tag{3}$$

We can write the solution of equation(3) in the form

$$S(y, \alpha, t) = W(y, \alpha) - \alpha t \tag{4}$$

We get

$$\frac{\partial S}{\partial y} = \frac{\partial W}{\partial y},$$

and $$\frac{\partial S}{\partial t} = -\alpha$$

Then eq. (3) takes the form

$$\frac{1}{2m}\left(\frac{\partial W}{\partial y}\right)^2 + mgy - \alpha = 0$$

or $$\frac{\partial W}{\partial y} = \sqrt{(2m)}\sqrt{(\alpha - mgy)} \tag{5}$$

or $$W = \sqrt{(2m)}\int \sqrt{(\alpha - mgy)}dy + c$$

where c is the constant of integration.

Thus eq. (4) can be written as given below

$$S = \sqrt{(2m)}\int \sqrt{(\alpha - mgy)}.dy + c - \alpha t$$

giving $\beta = \frac{\partial S}{\partial \alpha} = \sqrt{\left(\frac{m}{2}\right)}\int \frac{dy}{\sqrt{(\alpha - mgy)}} - t$

$$= \sqrt{\left(\frac{m}{2}\right)}\frac{2}{mg}\sqrt{(\alpha - mgy)} - t$$

or $$(\beta + t)^2 = \frac{1}{g^2}.\frac{2}{m}(\alpha - mgy)$$

gives $$y = -\frac{1}{2}g(\beta + t)^2 + \frac{\alpha}{mg} \tag{6}$$

We assume the initial conditions to be such that at t = 0

$$y = y_0 \text{ and } p = 0$$

Hence from equation (5), we obtain

$$p = \frac{\partial W}{\partial y} = \sqrt{(2m)}\sqrt{(\alpha - mgy)} = 0$$

giving $\alpha = mgy_0$, because $y = y_0$

After substituting above quantities in equation (6) ,we have

$$y = -\frac{1}{2}g(\beta + t)^2 + y_0 \tag{7}$$

Further at $t = 0, y = y_0$ so that from equation (7) we conclude that $\beta = 0$ and hence the equation of path of a particle falling vertically under the gravity becomes

$$y = -\frac{1}{2}gt^2 + y_0$$

Example 10.4 Consider the two-dimensional anisotropic harmonic oscillator. Mass of the oscillating body is m and k_x and k_y be the spring constants in the x -and y -directions, respectively, By using Hamilton Jacobi method, solve the problem. Also obtain the solution for isotropic oscillator.

Sol. The Hamiltonian is

$$E = \frac{1}{2m}\left(p_x^2 + p_y^2 + m^2\omega_x{}^2x^2 + m^2\omega_y^2y^2\right)$$

here $\omega_x = \sqrt{\frac{k_x}{m}}$ *and* $\omega_y = \sqrt{\frac{k_y}{m}}$.

Because the coordinates and momenta separate into two distinct sets, the principal function can be written as a sum of the characteristic function for each pair. we solve the $y-$ functional dependency first i.e

$$S\left(x, y, \alpha, \alpha_y, t\right) = F_x\left(x, \alpha\right) + F_y\left(y, \alpha_y\right) - \alpha t \tag{1}$$

The Hamilton- Jacobi equation takes the form

$$\frac{1}{2m}\left[\left(\frac{\partial W}{\partial x}\right)^2 + m^2\omega_x^2x^2 + \left(\frac{\partial W}{\partial y}\right)^2 + m^2\omega_y^2y^2\right] = \alpha \tag{2}$$

Because the variables are separated ,the y part of the eq.(2) must be equal to a constant, which we assume α_y

$$\frac{1}{2m}\left(\frac{\partial W}{\partial y}\right)^2 + \frac{1}{2}m\omega_y^2y^2 = \alpha_y \tag{3}$$

From eq.(2),(3)

$$\frac{1}{2m}\left(\frac{\partial W}{\partial x}\right)^2 + \frac{1}{2}m\omega_x^2x^2 = \alpha_{x,} \tag{4}$$

here we use $\alpha - \alpha_y = \alpha_x$ by symmetry of Eqs.(3) and (4) each equation has a solution

$$x=\sqrt{\frac{2\alpha_x}{m\omega_x^2}}\sin\left(\omega_x t+\beta_x\right)$$

$$p_x=\sqrt{2m\alpha_x}\cos\left(\omega_x t+\beta_x\right)$$

$$y=\sqrt{\frac{2\alpha_y}{m\omega_y^2}}\sin\left(\omega_y t+\beta_y\right)$$

$$p_y=\sqrt{2m\alpha_y}\cos\left(\omega_y t+\beta_y\right) \tag{5}$$

Here $\beta_i's$ are phase constants and the total energy is

$$E=\alpha_x+\alpha_y=\alpha,$$

, we consider two dimensional isotropic harmonic oscillator i.e.

$$k_x=k_y=k \text{ and } \omega_x=\omega_y=\omega,$$

In Polar coordinates

$$x=r\cos\theta \quad , \quad r=\sqrt{x^2+y^2}$$

$$y=r\sin\theta \quad , \quad \theta=\tan^{-1}\frac{y}{x}$$

$$\boxed{p_x=m\dot{x}} \qquad \boxed{p_y=m\dot{y}}$$

$$\boxed{p_r=m\dot{r}} \qquad \boxed{p_\theta=mr^2\dot{\theta}} \tag{6}$$

The Hamiltonian can be written as

$$E=\frac{1}{2m}\left(p_r^2+\frac{p_\theta^2}{r^2}+m^2\omega^2r^2\right) \tag{7}$$

The principle function can be written in terms the angular coordinate θ.

$$\begin{aligned} S\left(r,\theta,\alpha,\alpha_\theta\right) &= W_r\left(r,\alpha\right)+W_\theta\left(\theta,\alpha_\theta\right)-\alpha t \\ &= W_r\left(r,\alpha\right)+\theta\alpha_\theta-\alpha t, \end{aligned} \tag{8}$$

Since a cyclic coordinate q_i always has the characteristic function component $W_{q_i}=q_i\alpha_i$ The canonical momentum p_θ is calculated from the generating function

$$p_\theta = \frac{\partial F_\theta}{\partial \theta} = \alpha\theta$$

Using this p_θ in eqs.(7) and (8), $W_r(r,\alpha)$ satisfies

$$\frac{1}{2}\left(\frac{\partial W_r}{\partial r}\right)^2 + \frac{\alpha_\theta^2}{2mr^2} + \frac{1}{2}m\omega^2 r^2 = \alpha$$

We write the Cartesian coordinate solution for these conditions as

$$x = \sqrt{\frac{2\alpha}{m\omega^2}}\sin(\omega t + \beta)$$

$$p_x = \sqrt{2m\alpha}\cos(\omega t + \beta)$$

$$y = \sqrt{\frac{2\alpha}{m\omega^2}}\sin\omega t$$

$$p_y = \sqrt{2m\alpha}\cos\omega t$$

and using these ,we get in polar coordinates

$$r = \sqrt{\frac{2\alpha}{m\omega^2}}\sqrt{\sin^2\omega t + \sin^2(\omega t + \beta)}\ ,$$

$$p_r = m\dot{r},$$

and $$\theta = \tan^{-1}\left[\frac{\sin\omega t}{\sin(\omega t + \beta)}\right]\ ,$$

$$p_\theta = mr^2\dot{\theta}$$

10.6 Summary

We have set up the first order partial differential equation known as Hamilton-Jacobi equation. We have found a complete integral of H-J equation. We have used H-J equation in solving Kepler's problem and simple harmonic oscillator problems.

10.7 Glossary

***Anisotropic*:** (Of an object or substance) having a physical property which has different value when measured in different direction ; (Of a property or phenomenon) varying in magnitude according to the direction of measurement

***Arbitrary*:** (Of a constant or other quantity) of unspecified value.

10.8 Answers to Self Learning Exercise

Ans.1: $\frac{\partial S}{\partial t} + H(q, p, t) = 0$

10.9 Exercise

Q.1 Write down the the Hamiltonian of a particle in spherical coordinates

Q.2 Explain the method of "separating the variables" for obtaining a complete integral of the Hamilton-Jacobi equation.

Q.3 Express the Hamiltonian of a particle in spherical coordinates. Assume the potential energy of the particle is $U = a(r) + \frac{b(\theta)}{r^2}$, find the complete integral of the H-J equation.

Q.4 Solve the Kepler's problem by the method of separation of variables in the Hamilton-Jacobi equation.

10.10 Answers to Self Learning Exercise

Ans.1: $H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta} \right) + U(r, \theta, \phi)$

References and Suggested Readings

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UNIT-11

The Statistical Basis of Thermodynamics

Structure of the Unit

11.0 Objectives

11.1 The macroscopic and the microscopic states

11.2 Relation between statistics and thermodynamics

11.3 Physical significance of various statistical quantities

11.4 Self learning exercise I

11.5 Classical ideal gas

11.6 The entropy of mixing, *Sackur-Tetrode* equation

11.7 Correct enumeration of the microstates

11.8 Self Learning Exercise II

11.9 Summary

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11.11 Answer to self learning exercises

11.12 Exercise

References and Suggested Readings

11.0 Objectives

In this unit we briefly discuss the statistical basis of thermodynamics and understand the physical significance of various statistical quantities.

11.1 The Macroscopic and the Microscopic States

From the seventeenth century onward it was realized that material systems could often be described by a small number of descriptive parameters that were related to one another in simple law like ways.

These parameters referred to geometric, dynamical and thermal properties of matter.

The main aim of this chapter is the investigation of general properties of the macroscopic systems with a large number of degrees of dynamically freedom (with $N \sim 10^{20}$ particles).

From the mechanical point of view, such systems are very complicated. But in the usual case only a few physical parameters, say temperature, the pressure and the density, are measured, by means of which the "state'' of the system is specified.

A state defined in this crude manner is called a macroscopic state or thermodynamic state. On the other hand, from a dynamical point of view, each state of a system can be defined, at least in principle, as precisely as possible by specifying all of the dynamical variables of the system. Such a state is called a microscopic state.

A macrostate is defined by values of the macroscopic parameters which can be controlled. For an isolated system, these are N, E and V.

A microstate is a set of positions and momenta which are consistent with the prescribed energy E, volume V and particle number N.

The quantity $\Omega\ (N;V;T)$is the number of microstates which are consistent with a particular macrostate.

11.2 Relation between Statistics and Thermodynamics

Two systems, 1 and 2 are in thermal contact, i.e, their respective volumes and particle numbers are fixed, but they can exchange energy. The total energy of the system is fixed E. In that case, the total system has a number of microstates which, for a particular partitioning of the total energy (E_1;E_2), is given by

$$\Omega(N_1,V_1,E_1,N_2,V_2,E_2)= \Omega(N_1,V_1,E_1)\ \Omega(N_2,V_2,E_2)$$

With constant $E=E_1+E_2$.

The Particle numbers are very large, so the quantity Ω is sharply peaked around its maximum as a function of E_1. Therefore, the most likely value of E_1 is equal to the average value of E_1. We find the most likely value by putting

$$\frac{\partial ln\Omega(N_1,V_1,E_1,N_2,V_2,E_2)}{\partial E_1}$$

equal to zero. This lead to the condition for equilibrium

$$\frac{\partial ln\Omega(N_1,V_1,E_1)}{\partial E_1} = \frac{\partial ln\Omega(N_2,V_2,E_2)}{\partial E_2}$$

We have

$$\boxed{\beta = \frac{1}{k_B T}}$$

and

$S = k_B ln\Omega(N,V,E)$ Where S is entropy and T is temperature.

Similar, we can study two systems which are not only in thermal equilibrium (which can exchange thermal energy) but also in mechanical equilibrium (which can change their volumes V_1 and V_2 while keeping the sum $V_1 + V_2 = V$ constant). We then find that, in addition to the temperature, the quantity η is the same in both systems, i.e. pressure and temperature are the same in both.

Where

$$\boxed{\eta = \frac{P}{k_B T} = \frac{\partial \ln \Omega(N,V,E)}{\partial V}}$$

and if the system can exchange particles, then the quantity ζ is the same in both.

$$\boxed{\varsigma = -\frac{\mu}{k_B T} = \frac{\partial \ln \Omega(N,V,E)}{\partial N}}$$

The quantity μ is known as the ***chemical potential.***

In above discussion, P and μ are thermodynamic quantities. We have derived relations between these and the fundamental quantity $\Omega(N;V;E)$ which has a well-defined meaning in statistical physics (as do N,V and E) by using the relation

$$\boxed{S = k_B ln\Omega}$$

and thermodynamic relation

$$\boxed{dE = TdS - PdV + \mu dN}$$

From above equations the following relations can be derived straightforwardly:

$$\boxed{P = -\left(\frac{\partial E}{\partial V}\right)_{N,S}}$$

$$\boxed{\mu = \left(\frac{\partial E}{\partial N}\right)_{V,S}}$$

$$\boxed{T = \left(\frac{\partial E}{\partial S}\right)_{N,V}}$$

Other Thermodynamic quantities

- Helmholtz free energy

  $$\boxed{A = E - TS}$$

- Gibbs free energy

  $$\boxed{G = A + PV = E - TS + PV = \mu N}$$

- Enthalpy

  $$\boxed{H = E + PV = G + TS}$$

- Specific heat at constant volume

  $$\boxed{C_V = T\left(\frac{\partial S}{\partial T}\right)_{N,V} = \left(\frac{\partial E}{\partial T}\right)_{N,V}}$$

- Specific heat at constant pressure

  $$\boxed{C_P = T\left(\frac{\partial S}{\partial T}\right)_{N,P} = \left(\frac{\partial H}{\partial T}\right)_{N,P}}$$

11.3 Physical Significance of Various Statistical Quantities

The grand canonical function can be written as

$$Z = \sum_{N=0}^{\infty} e^{\beta\mu N}\, \Omega(N,V,T)$$

Where $\Omega(N,V,T)$ is the canonical partition function, which is related to Helmholtz free energy A as

$$\Omega(N,V,T) = e^{-A/k_B T}$$

where

$$A=\mu N - PV$$

and hence

$$z = \sum_{N=0}^{\infty} e^{\beta\mu N}\, e^{-A/k_B T}$$

The sum $e^{-A/k_B T} e^{\beta\mu N}$ will be very sharply peaked near the equilibrium value of N, so that we may replace the sum by the sum at its peak value.

$$k_B T \ln Z = \mu N - A = \mu N - E + TS$$

using thermodynamics relation

$$E=TS-PV+\mu N$$

then

$$k_B T \ln Z = PV = k_B T\, q$$

Note that we have been a bit sloppy in replacing the sum over N by its maximum value (we should have included a width here). However, this only leads to an additive constant in the relation between $\mu N - A$ and $k_B T \ln Z$, which can be fixed by noting that for $N = 0$, the right hand side should vanish, and the result obtained turns out to be correct.

Let us now calculate the average value of N using the density function:

$$N = \frac{\sum_{N=0}^{\infty} N e^{-\beta\,\mu\,N}\, e^{-A/k_B T}}{\sum_{N=0}^{\infty} e^{-\beta\,\mu\,N}\, e^{-A/k_B T}} \quad N = k_B T\, \frac{\partial\, q(\mu, V, T)}{\partial \mu}$$

The energy can be obtained as

$$U = k_B T^2 \left(\frac{\partial\, q(Z, V, T)}{\partial T}\right)_{Z,V}$$

Note that in the derivative with respect to T, Z is kept constant (though it depends on T).

The relations with thermodynamic quantities can most easily be formulated as

$$N = k_B T^2 \left(\frac{\partial\, k_B T \ln Z}{\partial \mu}\right)_{V,T}$$

$$P = \left(\frac{\partial\, k_B T \ln Z}{\partial V}\right)_{\mu,T}$$

$$S = \left(\frac{\partial\, k_B T\, ln\, Z}{\partial T}\right)_{\mu,V}$$

N, V are respectively the number of particles and the volume of the system. We let both quantities go to infinity, while keeping the ratio $n=N/V$ constant. In that case, quantities which scale linearly with *V* (or *N*) are called extensive, while quantities which do not scale with *V* (or *N*) are called intensive.

11.4 Self Learning Exercise- I

Section A :Very Short Answer Type Questions

Q.1 Define macroscopic states?

Q.2 Define microscopic states?

Section B: Short Answer Type Questions

Q.3 Explain the Difference between macroscopic and microscopic properties?

Q.4 Write down the macro and microscopic parameters?

Q.5 Give the definition of entropy in statistical physics.

Q.6 Derive Stirling's approximation for large *n*

ln *n!*=*n* ln *n*-*n*

by approximation ln*n!* by an integral.

11.5 Classical Ideal Gas

If *N* particles in a volume *V* do not interact, the number of ways the particles can be distributed in that volume scales as V^N

i.e. $\Omega = V^N$

Therefore

$$\frac{P}{T} = k_B \left(\frac{\partial\, ln\Omega(N,E,V)}{\partial V}\right)_{N,E} = k_B \frac{N}{V}$$

For a more consistent derivation of the entropy, we consider a particular example: a quantum mechanical system consisting of particles within a cubic volume $V = L^3$ and with total energy *E*.

The particles have wave functions

$$\psi(x;y;z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right) sin\left(\frac{n_y \pi y}{L}\right) sin\left(\frac{n_z \pi z}{L}\right)$$

With energy

$$E = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right) = \frac{\hbar^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$

The number Ω *(N,V,E)* is the number of points on the surface of a sphere with radius $\frac{2mE}{\hbar^2}$ in a grid with unit grid constant in 3N dimensions. But it might occur that none of the grid points lies precisely on the sphere (in fact that is rather likely!) .In order to obtain sensible physics, we therefore consider the number of points in a spherical shell of radius $\frac{2mE}{\hbar^2}$ and thickness much smaller than the radius (but much larger than the grid constant). The number of points in such a grid is called Γ

The surface of a sphere of radius *r* in *3N* dimensions is given by

$$\frac{2\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2}-1\right)!} r^{3N-1}$$

Total number of microstates can now be written as

$$\Omega(E,N,V) = \frac{\frac{V^N}{\hbar^{3N}} 2\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2} - 1\right)!} (2mE)^{\frac{3N-1}{2}} \sqrt{\left(\frac{m}{2E}\right)} \Delta E$$

$$= \frac{\frac{V^N}{\hbar^{3N}} (2\pi mE)^{\frac{3N}{2}}}{\left(\frac{3N}{2} - 1\right)!} \frac{\Delta E}{E}$$

Entropy of the gas can now be written as

$$S(N;V;E) = k_B \, log\Omega$$

$$= k \, log \frac{\frac{V^N}{\hbar^{3N}} (2\pi mE)^{\frac{3N}{2}}}{\left(\frac{3N}{2} - 1\right)!} \frac{\Delta E}{E}$$

$$= Nk_B \, log\left(\frac{V}{\hbar^3} (2\pi mE)^{\frac{3}{2}}\right) - k_B log\left(\frac{3N}{2} - 1\right)! + k_B log \frac{\Delta E}{E}$$

For a macroscopic gas, N is very large, of the order of 10^{23}, and it makes sense to use the Stirling formula $log(n!) \approx n \, log(n) - n$. So we get

$log\ (3N/2-1)!\ \approx\ (3N/2-1)log(3N/2-1)-3N/2+1$

$\approx\ (3N/2-1)log(3N/2)-3N/2+1$

Entropy of the gas now takes the form

$$S(E,V,N) = Nk_B\ log\left(\frac{V}{\hbar^3}\ (2\pi mE)^{\frac{3}{2}}\right) - k_B\left(\frac{3N}{2} - 1\right) log\ \left(\frac{3N}{2}\right) + \frac{3Nk_B}{2} - k_B + k_B log\frac{\Delta E}{E}$$

$$= Nk_B\ log\left(\frac{V}{\hbar^3}\left(\frac{2\pi mE}{(3N/2)}\right)^{\frac{3}{2}}\right) + \frac{3Nk_B}{2} + \left\{k_B\ log\left(\frac{3N}{2}\right) - k_B + k_B\ log\frac{\Delta E}{E}\right\}$$

In the equation above, the terms in the curly brackets are all much smaller than the other terms, which are at least of order N, and hence can be neglected to yield

$$S = Nk_B \log\left[\frac{V}{\hbar^3}(4\pi mE/3N)^{3/2}\right] + \frac{3}{2}Nk_B$$

It can be shown that an extra term containing the thickness of the shell is negligibly small in the thermodynamic limit. This expression can be inverted to yield the energy as a function of S, V and N:

$$E(S;V;N)\ = \frac{3\hbar^2 N}{4\pi m V^{\frac{2}{3}}} \exp\left(\frac{2S}{3Nk_B} - 1\right)$$

This equation together with

$$T^{-1} = \left(\frac{\partial S}{\partial E}\right)_{N,V}$$

leads to the relations

$$E\ = \frac{3}{2}Nk_BT, C_V = \frac{3}{2}Nk_B;\ C_p = \frac{5}{2}Nk_B$$

From the last two relations, we find for the ratio of the two specific heats

$$C_p/C_v = \frac{5}{3}$$

It can be verified that the change in entropy during an isothermal change of a gas (i.e. N and T constant) is

$$S_f - S_i = Nk_B \ln\left(\frac{V_f}{V_i}\right)$$

Furthermore, during an adiabatic change (i.e. *N* and *S* constant),

$$PV^{\gamma} = const$$
$$TV^{\gamma-1} = const$$

with $\gamma = 5/3$.

The work done by such an adiabatic process is given by

$dE = -PdV = -(2E/3V)dV$

11.6 The Entropy of Mixing, *Sackur-Tetrode* Equation

Mixing of two different gases is an irreversible process. It should thus lead to an increase in entropy. Let us check that out in our expression for entropy of an ideal gas. Let there be a box of volume V, which is partitioned. Let there be two dfferent, but similar, gases in the two partitions, at the same temperature and pressure. We remove the partition, and allow the gases to mix.

Before mixing, the initial entropy of the combined system, before mixing, is just the sum of the entropies of the two gases:

$$S = N_1 k_B \log\left[\frac{V_1}{\hbar^3}(4\pi m_1 E_1/3N_1)^{3/2}\right] + \frac{3}{2}N_1 k_B + N_2 k_B \log\left[\frac{V_2}{\hbar^3}(4\pi m_2 E_2/3N_2)^{3/2}\right] + \frac{3}{2}N_2 k_B$$

After the partition is removed, the energy, pressure, temperature of the gases will not change, as they were already at same temperature and pressure. The only difference is that now volume V is available to both the gases. The final entropy, after mixing, looks like

$$S_F = N_1 k_B \log\left[\frac{V}{\hbar^3}(4\pi mE/3N)^{3/2}\right] + \frac{3}{2}N_1 k_B + N_2 k_B \log\left[\frac{V}{\hbar^3}(4\pi mE/3N)^{3/2}\right] + \frac{3}{2}N_2 k_B$$

$$= (N_1 + N_2) k_B \log\left[\frac{V}{\hbar^3}(4\pi mE/3N)^{3/2}\right] + \frac{3}{2}(N_1 + N_2)k_B$$

$$= Nk_B \log\left[\frac{V}{\hbar^3}(4\pi mE/3N)^{3/2}\right] + \frac{3}{2}Nk_B$$

The change in entropy is given by

$$\Delta S = k_B[N_1 \ln\frac{V_1 + V_2}{V_1} + N_2 \ln\frac{V_1 + V_2}{V_2}]$$

Clearly, the entropy increases after mixing of the two gases, which is what one would expect. ΔS is called the entropy of mixing. However, there is a problem. If

the two gases were identical, removing the partition should not have any effect. In this case $E_1/N_1 = E_2/N_2 = E/N$. The final entropy in the case of identical gases, is given by

$$S_F = N_1 k_B \ln\left[\frac{V}{\hbar^3}\left(\frac{4\pi m_1 E_1}{3N_1}\right)^{\frac{3}{2}}\right] + \frac{3}{2}N_1 k_B + N_2 k_B \, ln\left[\frac{V}{\hbar^3}\left(\frac{4\pi m_2 E_2}{3N_2}\right)^{\frac{3}{2}}\right] + \frac{3}{2}N_2 k_B$$

$$= (N_1 + N_2) k_B \, log\left[\frac{V}{\hbar^3}(4\pi m E/3N)^{3/2}\right] + \frac{3}{2}(N_1 + N_2) k_B$$

$$= N k_B \, log\left[\frac{V}{\hbar^3}(4\pi m E/3N)^{3/2}\right] + \frac{3}{2} N k_B$$

For the case of same gas in the two parts, removing the partition is a reversible process, because one can reinsert the partition later, and one will not be able to make out if the partition was removed before. Hence, the change in entropy on removing the partition should be zero. The fact that for entropy yields a non-zero entropy of mixing for identical gases, is called ***Gibb's paradox.***

Gibb's empirically realized that while counting the number of microstates, if one divides the number of microstates by N!, the paradox disappears. How concluded that our counting of microstates must be thus wrong. The way we have counted the microstates, interchanging two particles gives one a new microstate. However, from quantum mechanics we know that elementary particles and atoms should be treated as identical particles. So, the way we have counted the microstates, we have done an overcounting by assuming the particles to distinguishable. So, we must divide by N! to correct for it.

$$\Omega(E, N, V) = \frac{\frac{V^N}{\hbar^{3N}}(2\pi m E)^{\frac{3N}{2}}}{N!\left(\frac{3N}{2} - 1\right)!}\frac{\Delta E}{E}$$

Using Stirling's approximation for N!, we have to subtract k[N log(N)−N] to obatin the correct expression for entropy

$$S(E, N, V) = N k_B \, log\left[\frac{V}{\hbar^3}(4\pi m E/3N)^{3/2}\right] + \frac{5}{2} N k_B$$

This is called the Sackur-Tetrode equation, and describes the entropy of a classical (monatomic) ideal gas. It is named for Hugo Martin Tetrode (1895-1931) and Otto Sackur (1880-1914), who developed it independently as a solution of Boltzmann's gas statistics and entropy equations, at about the same time in 1912.

The entropy of two gases before mixing is now given by

$$S = N_1 k_B \, log\left[\frac{V_1}{\hbar^3}\left(\frac{4\pi m_1 E_1}{3N_1}\right)^{3/2}\right] + \frac{5}{2}N_1 k_B + N_2 k_B \, log\left[\frac{V_2}{\hbar^3}\left(\frac{4\pi m_2 E_2}{3N_2}\right)^{3/2}\right] + \frac{5}{2}N_2 k_B$$

If the two gases are the same, $V_1/N_1 = V_2/N_2 = V/N$ and energy per particle is also same, if they are at the same temperature and pressure, $E_1/N_1 = E_2/N_2 = E/N$. So, the above equation reduces to

$$S = N_1 k_B \, log\left[\frac{V_1}{\hbar^3}\left(\frac{4\pi m_1 E_1}{3N_1}\right)^{3/2}\right] + \frac{5}{2}N_1 k_B + N_2 k_B \, log\left[\frac{V_2}{\hbar^3}\left(\frac{4\pi m_2 E_2}{3N_2}\right)^{3/2}\right] + \frac{5}{2}N_2 k_B$$

$$= (N_1 + N_2)k_B \, log\left[\frac{V}{\hbar^3}\left(\frac{4\pi m_1 E}{3N}\right)^{3/2}\right] + \frac{5}{2}(N_1 + N_2)k_B$$

$$= N k_B \, log\left[\frac{V}{\hbar^3}\left(\frac{4\pi m_1 E}{3N}\right)^{3/2}\right] + \frac{5}{2}N k_B$$

which is the equation for the entropy of the gas of N particles in a volume V, that is, the gas after mixing. So, for the case of same gas, mixing has no effect.

11.7 The"Correct"Enumeration of the Microstates

The entropy of an N-particle system by an amount *k ln N!,* which implies an ad hoc reduction in the number of microstates accessible to the system by a factor N!, was able to correct the unphysical features of some of our former expressions. The physical reason for doing so is that the particles constituting the given system are not only identical but also *indistinguishable*; accordingly, it is unphysical to label them as No. 1, No. 2, No. 3, and so on and to speak of their being *individually* in the various single-particle states ε_i . All we can sensibly speak of is their distribution over the states ε_i by *numbers*, that is, n_1 particles being in the state "1, n_2 in the state "2, and so on. Thus, the correct way of specifying a microstate of the system is through the distribution numbers n_i and not through the statement as to "which particle is in which state." To elaborate the point, we may say that if we consider two microstates that differ from one another merely in an interchange of two particles in different energy states, then according to our original mode of counting we would regard these microstates as distinct; in view of the

indistinguishability of the particles, however, these microstates are not distinct (for, physically, there exists no way whatsoever of distinguishing between them).

Now, the total number of permutations that can be effected among N particles, distributed according to the set n_i, is

$$\frac{N!}{n_1!\, n_2! \ldots .}$$

If our particles were distinguishable, then all these permutations would lead to "distinct" microstates. However, in view of the indistinguishability of the particles, these permutations must be regarded as leading to one and the same thing; consequently, for *any* distribution set n_i, we have one, and only one, distinct microstate. Since factor itself depends on the numbers n_i constituting a particular distribution set and for a given macrostate there will be many such sets, there is no straightforward way to "correct down" the number of microstates computed on the basis of the classical concept of "distinguishability" of the particles.

The recipe of Gibbs clearly amounts to disregarding the details of the numbers n_i and slashing the whole sequence of microstates by a *common* factor $N!$ this is correct for situations in which all N particles happen to be in different energy states but is certainly wrong for other situations. We must keep in mind that by adopting this recipe we are still using a spurious *weight factor*,

$$w\{n_i\} = \frac{1}{n_1!\, n_2! \ldots}$$

for the distribution set n_i whereas in principle we should use a factor of *unity*, irrespective of the values of the numbers n_i. Nonetheless, the recipe of Gibbs does correct the situation in a gross manner, though in matters of detail it is still inadequate. In fact, it is only by taking weight factor to be equal to unity (or zero) that we obtain true *quantum statistics*!

We thus see that the recipe of Gibbs corrects the enumeration of the microstates, as necessitated by the indistinguishability of the particles, only in a gross manner. Numerically, this would approach closer and closer to reality as the probability of the n_i being greater than 1 becomes less and less. This in turn happens when the given system is at a sufficiently high temperature (so that many more energy states become accessible) and has a sufficiently low density (so that there are not as many particles to accommodate). ***It follows that the "corrected" classical statistics***

represents truth more closely if the expectation values of the occupation numbers n_i are much less than unity:

$$< n_i > \ll 1$$

11.8 Self Learning Exercise -II

Short Answer Type Questions

Q.1 If $S=-k_B N[p \ln(p)+(1-p)\ln(1-p)]$,

by doing a variation w.r.to p find the value of p that gives the maximum entropy. Demonstrate that it is a maximum by showing that the second derivative w.r.to p is negative.

Q.2 Why is the ideal gas law still a good starting point for high temperature gases, even though a non-interacting gas is non-ergodic ?

Q.3 Study the statistical mechanics of an extreme relativisitic gas characterized by the single-particle energy states

$$\varepsilon(n_x, n_y, n_z) = \frac{hc}{2L}\left(n_x^2 + n_y^2 + n_z^2\right)^{\frac{1}{2}}$$

Show that the ratio C_P/C_V in this case is 4/3, instead of 5/3.

Q.4 Calculate the probability P_1 of finding an ideal gas in the macrostate where all the molecules are in the leftmost 99% of the container; there are 100 molecules in the container.

Q.5 Derive the Sackur-Tetrode equation.

11.9 Summary

The unit starts with the introduction of macroscopic and the microscopic states followed by physical significance of various statistical quantities. In this unit we also discussed Classical ideal gas, the entropy of mixing, *Sackur-Tetrode* equation and"correct"enumeration of the microstates.

11.10 Glossary

Macroscopic: Pertaining to aspects of a system which can be measured classically, such as temperature, pressure etc; containing very large numbers of atoms.

Macrostate: The current disposition of the system defined in terms of macroscopic

variables. Also (in classical thermal physics) state.

Microscopic: Pertaining to the underlying quantum state of a system.

Microstate :The state of the system defined in terms of the current behaviour of all the constituent atoms. NOT "the state of a very small system"! Also quantum state.

Enthalpy H (in Joule): H=U+PV, where U is the internal energy, P pressure and V volume. Its change gives the heat at constant pressure when there is no other work.

Entropy S (in J/K): is a thermodynamic quantity that expresses the degree of disorder or randomness in a system at the molecular level

Helmholtz energy A (in J): defined as A=U−TS, where U is the internal energy, T is the thermodynamic temperature and S is the entropy. The change in Helmholtz energy at constant volume and temperature gives the maximal work available. In a closed system at constant volume and temperature the Helmholtz energy decreases during a spontaneous process.

Gibbs energy G (in J): defined as G=H−TS, where H denotes enthalpy, T the thermodynamic temperature and S the entropy. The change in Gibbs energy at constant pressure and temperature gives the maximal work available. In a closed system at constant pressure and temperature the Gibbs energy decreases during a spontaneous process.

Ideal gas: A gas whose pressure P, volume V, and temperature T are related by PV = nRT, where *n* is the number of moles of gas and R is the ideal gas law constant. Ideal gases have molecules with negligible size, and the average molar kinetic energy of an ideal gas depends only on its temperature. Most gases behave ideally at sufficiently low pressures.

11.11 Answer to Self Learning Exercises

Answer to Self Learning Exercise- I

Ans.1: A macrostate is defined by values of the macroscopic parameters which can be controlled. For an isolated system, these are *N, E* and *V*.

Ans.2: A microstate is a set of positions and momenta which are consistent with the prescribed energy *E*, volume *V* and particle number *N*.

Ans.3: The macroscopic level includes anything seen with the naked eye. The microscopic level includes atoms and molecules, things not seen with the naked eye. Both levels describe matter.

Ans.4: For an isolated system, macroscopic parameters are *N, E* and *V*.

and microstate parameters are positions and momenta which are consistent with the prescribed energy *E*, volume *V* and particle number *N*.

Ans.5: S=$k_B$lnΩ,

where k is Boltzmann's constant and Ω is the total number of microscopic states of the given macroscopic states.

Ans.6:

$$\ln n! = \sum_{m=1}^{n} \ln m \approx \int_{1}^{n} \ln x \, dx = n \ln n - n + 1 \approx n \ln n - n$$

(for large n)

Answer to Self Learning Exercise II

Ans.1: Taking a derivative with respect to p gives

$$\frac{\partial S}{\partial p} = -k_B N[lnp - \ln(1-p)]$$

The extrema occur at values of p = p* where this expression is zero, which yields p* = 1/2. To determine whether this is a minimum or maximum, we take the second derivative to find that,

$$\frac{\partial^2 S}{\partial p^2} = -k_B N\left[\frac{1}{p} + \frac{1}{1-\mathrm{p}}\right] = -k_B N$$

Since the second derivative is negative the extremum at p = 1/2 is a maximum. We have thus found the value of the probability at which the entropy is a maximum.

Ans.2: Even very small interactions can make the system chaotic. These interactions have little effect on the equilibrium thermodynamic behavior though they are critical to the transport properties.

Ans.3: (in the article)

Ans.4: The total number of microstates (multiplicity) accessible in this macrostate is $\Omega_1 = A(N,U)\cdot (0.99V)^{100}$, where V is the volume of the container, A(N,U) is some function of the energy and the number of particles. The total number of microstates in the most likely macrostate is $\Omega_0 = A(N,U)V^{100}$. Since all microstates of an isolated system are equally probable, we have

$P_1/P_0 = \Omega_1/\Omega_0 = 0.99^{100} = 0.366$

where P_1 and P_0 are the probabilities of the corresponding macrostates. If we take the probability of the most likely macrostate to be 1, then $p_1 = 0.366$

11.12 Exercise

Long Answer Type Questions

Q.1 Suppose that a differentiable function satisfies $f(xy) = f(x) + f(y)$ for all positive x and y. Show that $f(x) = k \ln(x)$

[Clues: (i) Take derivatives with respect to x and with respect to y.

(ii) If G(x) = G(y), x and y independent variables, then the function G(x) must be constant.

(iii) Set y = 1 in equation.]

Q.4 System 1 is in a macrostate with three corresponding microstates, labeled A, B, and C. System 2 is in a macrostate with four corresponding microstates, labeled α,β,γ and δ. How many microstates are accessible to the combined system consisting of system and system? List all such microstates.

Q.3 Show that the various expressions for the entropy of mixing, satisfy the following relations:

(a) For all N_1, V_1, N_2, and V_2,

$$\Delta S_{1\equiv 2} = \Delta S - \Delta S^* \geq 0$$

the equality holding when and only when $N_1/V_1 = N_2/V_2$.

(b) For a given value of $(N_1 + N_2)$,

$$\Delta S^* \leq (N_1 + N_2) k \ln 2,$$

the equality holding when and only when $N_1 = N_2$.

Q.4 If the two gases considered in the mixing process were initially at different temperatures, say T_1 and T_2, what would the entropy of mixing be in that case? Would the contribution arising from this cause depend on whether the two gases were different or identical?

Q.5 Show that for an ideal gas composed of monoatomic molecules the entropy change, between any two temperatures, when the pressure is kept constant is 5/3 times the corresponding entropy change when the volume is kept constant. Verify this result *numerically* by calculating the actual values of ΔS_P and ΔS_V per mole of an ideal gas whose temperature is raised from 300 K to 400 K.

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UNIT-12
Ensemble Theory

Structure of the Unit

12.0 Objectives

12.1 Phase space

12.2 Ensemble average

12.3 Liouville's theorem and its consequence

12.4 Self learning exercise- I

12.5 Microcanonical ensemble

12.6 Ensemble average

12.7 Phase trajectory of simple harmonic oscillator

12.8 Quantum states and phase space

12.9 Self Learning Exercise -II

12.10 Summary

12.11 Glossary

12.12 Answer to self learning exercises

12.13 Exercise

References and Suggested Readings

12.0 Objectives

After interacting with the material presented here students will be able to understand

1. The concept of phase space and ensemble average,
2. Liouville's theorem and its consequence
3. Microcanonical ensemble and ensemble average
4. Phase trajectory of simple harmonic oscillator
5. Quantum states and phase space

12.1 Phase Space

In general, phase space Γ is the space of a set of ordered numbers which describes the microscopic states of a many-particle system. For a classical system, one can describe the state of a system by a set of continuously varying variables corresponding to the generalized momenta and generalized coordinates of each particle. However, for quantum systems, the Heisenberg uncertainty principle forbids one to know the momentum and position of any single particle precisely. In this case, the quantum states of a particle can be prescribed by specifying the eigenvalues of a mutually commuting set of operators representing physical observables. The eigenvalues can be either continuous or discrete. Thus, the phase space for a quantum system can either consist of a set of discrete numbers or can consist of a set of continuous numbers, as in the classical case.

If N is the number of particles in the system, the definition of a microstate requires the specification of ***3N position coordinates*** $q_1, q_2, \cdots, q_{3N}$ ***and 3N momentum coordinates*** $p_1, p_2, \cdots, p_{3N}$. Geometrically, the set of coordinates (q_i, p_i), where i= 1, 2,.., 3N, may be regarded as a point in ***a space of 6N dimensions***. We refer to this space as the ***phase space***, and the phase point (q_i, p_i) as a representative point, of the given system.

The coordinates q_i and p_i are functions of the time t; the precise manner in which they vary with t is determined by the canonical equations of motion,

$$\dot{q}_i = \frac{\partial H(q_i, p_i)}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H(q_i, p_i)}{\partial q_i}$$

where i=1,2,..3N and $H(q_i, p_i)$ is the Hamiltonian of the system. Now, as time passes, the set of coordinates (q_i, p_i), which also defines the microstate of the system, undergoes a continual change. Correspondingly, our representative point in the phase space carves out a trajectory whose direction, at any time t, is determined by the velocity vector, which in turn is given by the equations of motion. It is not difficult to see that the trajectory of the representative point must remain within a limited region of the phase space. This is so because a finite volume V directly

limits the values of the coordinates q_i while a finite energy E limits the values of both the q_i and the p_i [through the Hamiltonian]. In particular, if the total energy of the system is known to have a precise value, say E, the corresponding trajectory will be restricted to the "hypersurface" $H(q_i,p_i)= E$ of the phase space; on the other hand, if the total energy may lie anywhere in the range $(E-\Delta/2,E+\Delta/2)$, the corresponding trajectory will be restricted to the "hypershell" defined by these limits.

12.2 Ensemble Average

Now, if we consider ***an ensemble of systems (i.e., the given system, along with a large number of mental copies of it) then, at any time t, the various members of the ensemble will be in all sorts of possible microstates;*** indeed, each one of these microstates must be consistent with the given macrostate that is supposed to be common to all members of the ensemble. In the phase space, the corresponding picture will consist of a swarm of representative points, one for each member of the ensemble, all lying within the "allowed" region of this space. The overall picture of this movement possesses certain interesting features, which are best appreciated in terms of what we call a density function $\rho(q,p;t)$.

This function is defined in such a way that at any time *t,* the number of representative points in the volume element $(d^{3N}q\ d^{3N}p)$ around the point (q,p) of the phase space is given by the product $\rho(q,p;t)\ d^{3N}q\ d^{3N}p$. Clearly, the density function $\rho(q,p;t)$ symbolizes the manner in which the members of the ensemble are distributed over various possible microstates at various instants of time. The statistical average of a given dynamical physical quantity $f(p,q)$ is equal:

$$< f >= \frac{\int f(p,q)\rho(q,p,t)d^{3N}qd^{3N}p}{\int \rho(q,p,t)d^{3N}qd^{3N}p}$$

The integrations in extend over the whole of the phase space**.**

An ensemble is said to be stationary if ρ does not depend explicitly on time, i.e. at all times

$$\frac{\partial \rho}{\partial t} = 0$$

Clearly, for such an ensemble the average value $< f >$ of any physical quantity $f(p,q)$ will be independent of time.

12.3 Liouville's Theorem and its Consequence

Consider an arbitrary "volume" ω in the relevant region of the phase space and let the "surface" enclosing this volume increases with time is given by

$$\frac{\partial}{\partial t}\int_{\omega} \rho \, d\omega$$

where $d\omega \equiv (d^{3N}q \; d^{3N}p)$. On the other hand, the net rate at which the representative points *''flow''* out of the volume ω (across the bounding surface σ) is given by

$$\int_{\sigma} \rho\vec{v}.\hat{n}d\sigma$$

here $\vec{v}$ is the vector of the representative points in the region of the surface element $d\sigma$. By the divergence theorem, we can be written as

$$\int_{\sigma} div(\rho\vec{v})d\omega$$

where

$$div(\rho\vec{v}) = \sum_{i=1}^{3N}\left\{\frac{\partial}{\partial q_i}(\rho\dot{q}_i) + \frac{\partial}{\partial p_i}\rho\dot{p}_i\right\}$$

Now, the necessary and sufficient condition that integral vanish for all arbitrary volumes ω is that the integrand itself vanish *everywhere* in the relevant region of the phase space. Thus, we must have

$$\boxed{\frac{\partial\rho}{\partial t} + div(\rho\vec{v}) = 0}$$

which is the equation of continuity for the swarm of the representative points.

$$\frac{\partial\rho}{\partial t} + \sum_{i=1}^{3N}\left\{\frac{\partial}{\partial q_i}(\rho\dot{q}_i) + \frac{\partial}{\partial p_i}(\rho\dot{p}_i)\right\} = 0$$

The last group of terms vanishes identically because, by the equations of motion, we have, for all i,

$$\frac{\partial\dot{q}_i}{\partial q_i} = \frac{\partial^2 H(q_i,p_i)}{\partial q_i \partial p_i} = \frac{\partial^2 H(q_i,p_i)}{\partial p_i \partial q_i} = -\partial\dot{p}_i/\partial p_i$$

Further, since $\rho \equiv \rho(q,p,t)$, the total time derivative of ρ, with the result that

$$\boxed{\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + [\rho, H] = 0}$$

known as Liouville's theorem. According to this theorem, the local density of the representative points, as viewed by an observer moving with a representative point, stays constant in time. Thus, the swarm of the representative points moves in the phase space in essentially the same manner as an incompressible fluid moves in the physical space.

12.4 Self Learning Exercise-I

Q.1 Explain Ensemble average.

Q.2 Prove Liouville theorem.

Q.3 What is meant by phase space ?

Q.4 Define classical and quantum phase space.

Q.5 Write down the equation of continuity.

12.5 Microcanonical Ensemble

In microcanonical ensemble the macrostate of a system is defined by the number of molecules N, the volume V, and the energy E. However, in view of the considerations expressed in previous section we may prefer to specify a range of energy values [(E−Δ/2) to (E+Δ/2)], rather than a sharply defined value *E*. With the macrostate specified, a choice still remains for the systems of the ensemble to be in *any one* of a large number of possible microstates. In the phase space, correspondingly, the representative points of the ensemble have a choice to lie *anywhere* within a "hypershell" defined by the condition

$$E - \frac{\Delta}{2} \leq H(q,p) \leq \mathrm{E} + \frac{\Delta}{2}$$

The volume of the phase space enclosed within this shell is given by

$$\omega = \int d\,\omega = \int d^{3N}\, q d^{3N} p$$

where the integration extends only over that part of the phase space and will be a function of the parameters *N*,*V*,*E*.

Now, the microcanonical ensemble is a collection of systems for which the density function ρ is, at all times, given by

$\rho(q,p)=\text{const}, \quad \text{if } E-\frac{\Delta}{2} \leq H(q,p) \leq E+\frac{\Delta}{2}$

$=0 \quad \text{Otherwise}$

12.6 Ensemble Average

The expectation value of the number of representative points lying in a volume element $d\omega$ of the relevant hypershell is simply proportional to $d\omega$. In other words, the *a priori* probability of finding a representative point in a given volume element $d\omega$ is the same as that of finding a representative point in an equivalent volume element $d\omega$ located

anywhere in the hypershell.

In these cases the ensemble average <f >, acquires a simple physical meaning. To see this, we proceed as follows.

$\langle f \rangle$ ***≡ the ensemble average of f***

= the time average of (the ensemble average of f)

Now, the processes of time averaging and ensemble averaging are completely independent, so the order in which they are performed may be reversed without causing any change in the value of $\langle f \rangle$. Thus

$\langle f \rangle$ = the ensemble average of (the time average of f).

Now, the time average of any physical quantity, taken over a sufficiently long interval of time, must be the same for *every* member of the ensemble. Therefore, taking an ensemble average thereof should be inconsequential, and we may write

$\langle f \rangle$ = the long time average of f

where the latter may be taken over *any* member of the ensemble. Furthermore, the longtime average of a physical quantity is all one obtains by making a measurement of that quantity on the given system, therefore, it may be identified with the value one expects to obtain through experiment. Thus, we finally have

$\langle f \rangle = f_{exp}$

This brings us to the most important result: the ensemble average of any physical quantity f is identical to the value one expects to obtain on making an appropriate measurement on the given system.

Example : A classical ideal gas composed of monatomic particles .

In the microcanonical ensemble, the volume ω of the phase space

accessible to the representative points of the (member) systems is given by

$$\omega = \int \ldots \int d^{3N}q d^{3N}p$$

where the integrations are restricted by the conditions that (i) the particles of the system are confined in physical space to volume V, and (ii) the total energy of the system lies between the limits (E—Δ/2) and (E+Δ/2). Since the Hamiltonian in this case is a function of the p_i alone, integrations over the q_i can be carried out straightforwardly; these give a

factor of V^N. The remaining integral is

$$\int \ldots \int_{(E-\frac{\Delta}{2})\le\sum_{i=1}^{3N}\frac{p_i^2}{2m}\le(E+\frac{\Delta}{2})} d^{3N}p = \int \ldots \int_{2m(E-\frac{\Delta}{2})\le\sum_{i=1}^{3N}y_i^2\le 2m(E+\frac{\Delta}{2})} d^{3N}y$$

which is equal to the volume of a 3N-dimensional hypershell, bounded by hyperspheres of radii

$$\sqrt{2m(E+\frac{\Delta}{2})}\ and\ \sqrt{2m(E-\frac{\Delta}{2})}$$

For Δ<<E, this is given by the thickness of the shell, which is almost equal to $\Delta(m/2E)^{1/2}$, multiplied by the surface area of a 3N-dimensional hypersphere of radius $\sqrt{2mE}$.

,By Integral calculus, we get

$$\omega \cong \frac{\frac{\Delta}{E}V^N(2\pi mE)^{\frac{3N}{2}}}{\left[\frac{3N}{2}-1\right]!}$$

and we obtain the desired correspondence, namely

$$\omega/\Gamma_{asymp} = \omega_0 = h^{3N}$$

Quite generally, if the system under study has N degrees of freedom,

the desired conversion factor is

$$\omega_0 = h^N$$

In the case of a single particle, N = 3; accordingly, the number of microstates available would asymptotically be equal to the volume of the allowed region of the phase space divided by h^3. Let Σp denote the number of microstates available to a free particle confined to volume V of the physical space, its momentum p being less than or equal to a

specified value P. Then

$$\sum p \approx \frac{1}{h^3}\int \ldots \int_{p \le P} d^3p d^3q = \frac{V}{h^3}\frac{4\pi}{3}p^3$$

from which we obtain for the number of microstates with momentum lying between p and $p+dp$

$$g(p)dp = \frac{d\sum p}{dp}dp \approx \frac{V}{h^3}\frac{4\pi}{3}p^2 dp$$

Expressed in terms of the particle energy, these expressions assume the form

$$\sum(E) \approx \frac{V}{h^3}\frac{4\pi}{3}(2mE)^{\frac{3}{2}}$$

and

$$a(\varepsilon)d\varepsilon = \frac{d\Sigma(\varepsilon)}{d\varepsilon}d\varepsilon \approx \frac{V}{h^3}2\pi(2m)^{\frac{3}{2}}\varepsilon^{\frac{1}{2}}d\varepsilon$$

12.7 Phase trajectory of Simple Harmonic Oscillator

In this section we consider a one-dimensional simple harmonic oscillator. The classical expression for the Hamiltonian of this system is

$$\boxed{H(q,p) = \frac{1}{2}kq^2 + \frac{1}{2m}p^2}$$

where k is the spring constant and m the mass of the oscillating particle. The space coordinate q and the momentum coordinate p of the system are given by

$$q = A\cos(\omega t + \varphi),$$

$$p = m\dot{q} = -m\omega A\sin(\omega t + \varphi)$$

A being the amplitude and ω the (angular) frequency of vibration given by

$$\omega = \sqrt{\left(\frac{k}{m}\right)}$$

The energy of the oscillator is a constant of the motion, and is given by

$$E = \frac{1}{2}m\omega^2 A^2$$

The phase-space trajectory of the representative point (q, p) of this system is determined by eliminating t between expressions for $q(t)$ and $p(t)$, we obtain

$$\frac{q^2}{\left(\frac{2E}{m\omega^2}\right)} + \frac{p^2}{2mE} = 1$$

which is ***an ellipse***, with axes proportional to $\sqrt{E}$ and hence area proportional to E; to be precise, the area of this ellipse is $2\pi E/\omega$.

Now, if we restrict the oscillator energy to the interval (E—Δ/2) and (E+Δ/2), its representative point in the phase space will be confined to the region bounded by elliptical trajectories corresponding to the energy values (E—Δ/2)and (E+Δ/2). The "volume" (in this case, the area) of this region will be

$$\int \dots \int_{\left(E-\frac{\Delta}{2}\right)\leq H(q,p)\leq \left(E+\frac{\Delta}{2}\right)} dpdq = \frac{2\pi\left(E+\frac{\Delta}{2}\right)}{\omega} - \frac{2\pi\left(E-\frac{\Delta}{2}\right)}{\omega}$$

$$= \frac{2\pi\Delta}{\omega}$$

According to quantum mechanics, the energy eigenvalues of the harmonic oscillator are given by

$$\boldsymbol{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$

where n=0,1,2,$\cdots$

In terms of phase space, one could say that the representative point of the system must move along one of the "chosen" trajectories, as shown in Figure; the area of the phase space between two consecutive trajectories, for which $\Delta = \hbar\omega$, is simply $2\pi\hbar^5$.

For arbitrary values of E and Δ, such that $E >> \Delta >> \hbar\omega$, the number of eigenstates within the allowed energy interval is very nearly equal to $\Delta/(\hbar\omega)$. Hence, the area

of the phase space equivalent to one eigenstate is, asymptotically, given by

$$\omega_0 = \left(\frac{2\pi\Delta}{\omega}\right) / \left(\frac{\Delta}{\hbar\omega}\right) = 2\pi\hbar = h$$

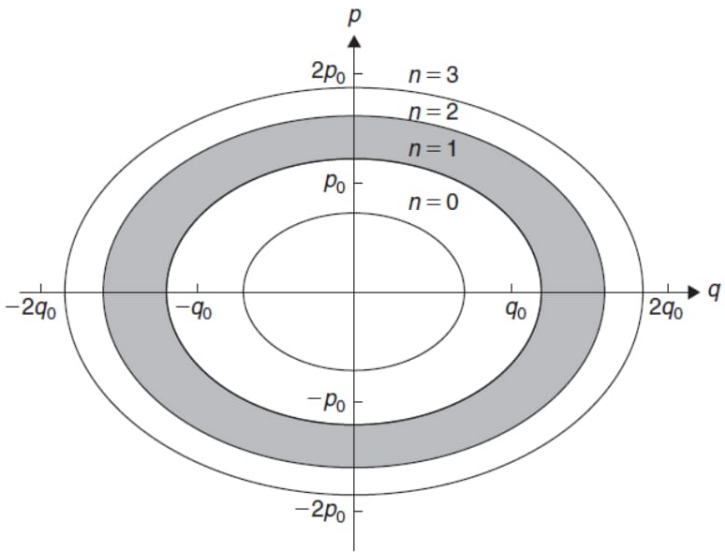


Figure: Eigenstates of a linear harmonic oscillator, in relation to its phase space.

12.8 Quantum States and Phase Space

According to Heisenberg uncertainty principle, we cannot specify simultaneously both the position and the momentum of a particle exactly. An element of uncertainty is inherently present and can be expressed as follows: assuming that all conceivable uncertainties of measurement are eliminated, even then, by the very nature of things, the product of the uncertainties Δq and Δp in the simultaneous measurement of the canonically conjugate coordinates q and p would be of order $\hbar$:

$$(\Delta q \Delta p)_{min} \sim \hbar$$

Thus, it is impossible to define the position of a representative point in the phase space of the given system more accurately than is allowed by above condition. In other words, around any point (q,p) in the (two-dimensional) phase space, there exists an area of order $\hbar$ within which the position of the representative point

cannot be pinpointed. In a phase space of 2N dimensions, the corresponding "volume of uncertainty" around any point would be of order $\hbar^N$. Therefore, it seems reasonable to regard the phase space as made up of elementary cells, of volume $\sim\hbar^N$, and to consider the various positions within such a cell as *nondistinct*. These cells could then be put into one-to-one correspondence with the quantum-mechanical states of the system.

It is, however, obvious that considerations of uncertainty alone cannot give us the *exact* value of the conversion factor ω_0. This could only be done by an *actual* counting of microstates on one hand and a computation of volume of the relevant region of the phase space on the other, as was done in the previous section.

We assume that $\omega_0=(zh)^N$

where z was supposed to be an unknown numerical factor. Comparing theoretical results with the experimental data on mercury, Tetrode found that z was very nearly equal to unity; from this he concluded that "it seems rather plausible that z is *exactly* equal to unity.

In the extreme relativistic limit, the same result was established by Bose (1924). In his famous treatment of the photon gas, Bose made use of Einstein's relationship between the momentum of a photon and the frequency of the associated radiation, namely

$$\boldsymbol{P=h\upsilon/c}$$

and observed that, for a photon confined to a three-dimensional cavity of volume V, the relevant "volume" of the phase space,

$$\int d^3\,qd^3p = V4\pi^2dp = V\left(\frac{4\pi h^3\upsilon^2}{c^3}\right)d\upsilon$$

would correspond exactly to the Rayleigh expression,

$$\boldsymbol{V\left(\frac{4\pi h^3\upsilon^2}{c^3}\right)d\upsilon}$$

for the number of normal modes of a radiation oscillator, *provided that* we divide phase space into elementary cells of volume h^3 and put these cells into one-to-one correspondence with the vibrational modes of Rayleigh.

It may, however, be added that a two-fold multiplicity of these states arises from the spin orientations of the photon (or from the states of polarization of the vibrational modes); this requires a multiplication of both expressions by a factor of 2, leaving the conversion factor h^3 unchanged.

12.9 Self Learning Exercise- II

Q.1 Derive the following expressions

(a) An asymptotic expression for the number of ways in which a given energy E can be distributed among a set of N one-dimensional harmonic oscillators, the energy eigenvalues of the oscillators being $\left(n+\frac{1}{2}\right)\hbar\omega$, n= 0, 1, 2,..

and

(**b**) The corresponding expression for the "volume" of the relevant region of the phase space of this system. Establish the correspondence between the two results, showing that the conversion factor ω_0 is precisely h^N.

Q.2 Why are the factors 1/N! and $1/h^{3N}$ introduced into the derivation of the partition function of the ideal classical gas?

Q.3 In the microcanonical ensemble, the total energy E is fixed. Counting the microstates having this energy, you can define the entropy $S(E)=k_B \ln\Omega(E)$, where $\Omega(E)$ is the number of microstates with energy E.

Q.4 Draw the phase trajectories of linear harmonic oscillator.

Q.5 What is meant by Microcanonical ensemble.

12.10 Summary

In this unit we discussed

- The concept of phase space and ensemble average,
- Liouville's theorem and its consequence
- Microcanonical ensemble and ensemble average
- Phase trajectory of simple harmonic oscillator
- Quantum states and phase space

12.11 Glossary

Harmonic oscillator: A harmonic oscillator is a physical system that, when displaced from equilibrium, experiences a restoring force proportional to the displacement. A harmonic oscillator that is displaced and then let go will oscillate sinusoidally. Examples from classical physics are a mass attached to a spring and a simple pendulum swinging through a small angle.

Steady-State: At steady state the concentrations if all species do not change even though at the same time the net reaction rates are non-zero. In contrast, at thermodynamic equilibrium, the net reaction rates are zero.

Thermodynamic Equilibrium: A chemical reaction is in thermodynamic equilibrium when the forward and reverse rates of the reaction are equal, that is the net reaction rate is zero.

Equilibrium: A system is in equilibrium when its macroscopic properties (temperature, pressure) are uniform and not changing with time.

Macroscopic: Pertaining to aspects of a system which can be measured classically, such as temperature, pressure etc; containing very large numbers of atoms.

Macrostate: The current disposition of the system defined in terms of macroscopic variables. Also (in classical thermal physics) state.

Microscopic: Pertaining to the underlying quantum state of a system

Microstate: The state of the system defined in terms of the current behavior of all the constituent atoms. NOT ``the state of a very small system"! Also quantum state.

12.12 Answer to Self Learning Exercises

Answer to Self Learning Exercise- I

Ans.1: Section 12.2

Ans.2: Section 12.3

Ans.3: Phase space Γ is the space of a set of ordered numbers which describes the microscopic states of a many-particle system.

Ans.4: For a classical system, one can describe the state of a system by a set of continuously varying variables corresponding to the generalized momenta

and generalized coordinates of each particle. However, the phase space for a quantum system can either consist of a set of discrete numbers or can consist of a set of continuous numbers, as in the classical case.

Ans.5 $\frac{\partial \rho}{\partial t} + div(\rho v) = 0$

Answer to Self Learning Exercise- II

Ans. 1:(a) Section 12.7

(b) If we consider a system of *N* harmonic oscillators along the same lines as mentioned in section 12.7, we arrive at the result: $\omega_0 = h^N$

Ans.2: The factor 1/N! is needed to account for the fact that when an integration is carried out over all phase space for N particles, all permutations of the particle identities is included. For identical particles this must be removed. The factor $1/h^{3N}$ takes account of the Heisenberg uncertainty principle which states that the smallest phase space volume that makes sense is $(\hbar/2)^3$. The fact that it is $1/h^3$ instead of $1/(\hbar/2)^3$ for each particle is to reproduce the high temperature behavior of quantum gases.

Ans.3: The partition function Z(E) is defined by

$$Z(E) = \sum_{\substack{\text{microstate} \\ i \text{ with} \\ \text{energy } E}} \omega_i$$

where ω_i is the weight of the microstate *i*. But in the ensemble, all microstates have the same probability, so ω_i is the same for all states and can be taken equal to 1. Therefore you end up with

$$Z(E) = \Omega(E)$$

The entropy $S(E)=k_B \ln Z(E)$ can therefore be seen as the thermodynamical potential in the microcanonical ensemble because you can obtain intensive quantities by derivation of S (like for instance 1/T=dS/dE).

Ans.4: In the section 12.7

Ans.5: This is the ensemble which allows you to calculate thermodynamics only using the knowledge that your system is made of a certain number of particles, which have a certain amount of energy between them. You then look at the ways this energy could be distributed between

the particles, and count them to get the entropy. This approach is really cool in that you can derive thermodynamic properties (like PV=nRT) instead of measuring them, but with a large number of particles the math gets messy.

12.13 Exercise

Long Answer Type Questions

Q.1 The energy levels of a quantum mechanical, one-dimensional anharmonic oscillator may be approximated as

$\varepsilon_n(n+1/2)\,\hbar\omega - x(n+1/2)^2\,\hbar\omega$

Find the heat capacity of N such oscillators to first order in x and fourth order in $u = \dfrac{\hbar\omega}{kT}$. Plot your result.

Q.2 In the microcanonical ensemble, the entropy for an ideal gas in the semiclassical limit is given by

$$S(E,V,N) = Nk\,log\left[\frac{V}{\hbar^3}\left(\frac{4\pi mE}{3N}\right)^{3/2}\right] + \frac{5}{2}Nk$$

Using the definition of thermodynamics temperature and pressure, derive the expressions for

(a) the internal energy of the ideal gas

(b) the equation of state

Q.3 Find the entropy S(E,V,N) of an ideal gas of N classical monatomic particles, with a fixed total energy E, combined in a *d*-dimensional box of volume V. Deduce the equation of state of this gas assuming that N is very large.

Q.4 For a collection of *N* three dimensional classical harmonic oscillator of frequency ω and fixed energy E. Compute S and the temperature T. Discuss whether the oscillator be treated as distinguishable or indistinguishable.

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UNIT-13
The Canonical Ensemble

Structure of the Unit

13.0 Objectives

13.1 Introduction

13.2 Equilibrium between a system and a heat reservoir

13.3 System in the canonical ensemble

13.4 Physical significance of the various statistical quantities in the canonical ensemble

13.5 Self learning exercise- I

13.6 Partition function

13.7 Classical system

13.8 Energy fluctuations in the canonical ensemble

13.9 The 'equipartition' and the 'virial' theorem

13.10 System of harmonic oscillators

13.11 The statistics of paramagnetism

13.12 Negative temperatures

13.13 Self learning exercise- II

13.14 Summary

13.15 Glossary

13.16 Answer to self learning exercise

13.17 Exercise

References and Suggested Readings

13.0 Objectives

After interacting with the material presented here students will be able to understand

- Details of canonical ensembles
- Concept of equipartition theorem, and virial theorem
- Statistics of paramagnetism,

13.1 Introduction

In the ***microcanonical ensemble the macrostate of the systems was defined through a fixed number of particles N, a fixed volume V, and a fixed energy E. The basic problem then consisted in determining the number Ω(N,V,E),*** or $\Gamma(N,V,E;\Delta)$, of distinct microstates accessible to the system. From the asymptotic expressions of these numbers, complete thermodynamics of the system could be derived in a straightforward manner. However, for most physical systems, the mathematical problem of determining these numbers is quite formidable. For this reason alone, a search for an alternative approach within the framework of the ensemble theory seems necessary.

Practically, the concept of a fixed energy (or even an energy range) for a system belonging to the real world does not appear satisfactory.

1. The total energy E of a system is hardly ever measured;
2. It is hardly possible to keep its value under strict physical control.

A far better alternative appears to be to speak of a fixed temperature T of the system - a parameter that is not only directly observable but also controllable (by keeping the system in contact with an appropriate "heat reservoir"). For most purposes, the precise nature of the reservoir is not very relevant, all one needs is that it should have an infinitely large heat capacity, so that, irrespective of energy exchange between the system and the reservoir, an overall constant temperature can be maintained. Now, if the reservoir consists of an infinitely large number of mental copies of the given system we have once again an ensemble of systems, it is an ensemble in which the macrostate of the systems is ***defined through the parameters N,V, and T. Such an ensemble is referred to as a canonical ensemble.***

13.2 Equilibrium between a System and a Heat Reservoir

Suppose we have large, isolated system which we divide up into a very small one and the rest. The small subsystem can exchange energy with the rest of the

system, but its volume and number of particles is constant. Consider a state r of the small subsystem with energy E_r. The subsystem in this state depends on the number of states which are accessible to the rest of the system (this is called the *heat bath*), and this number is given as $\Omega(E - E_r)$, where E is the energy of the total system. Therefore, the multiplicity of the state with energy E_r is

$$P_r = \Omega(E - E_r)$$

We know that Ω of the heat bath is given as $\exp(S/k_B)$. We then have

$$\begin{aligned} P_r &= \exp[S(E - E_r)/k_B] \\ &= exp\left\{\left[S(E) - \frac{\partial S(E)}{\partial E} E_r\right] / k_B\right\} \\ &= exp\left\{\left[S(E) - \frac{E_r}{T}\right] / k_B\right\} \end{aligned}$$

so that we obtain

$$\boxed{P_r = P(E_r) \propto \exp(-E_r / k_B T)} \text{ with } \boxed{\beta = 1/k_B T}$$

P_r is the Boltzmann distribution function.

As the subsystem is very small in comparison with the total system, its temperature will be determined by the later. Therefore the temperature of the subsystem will be a control parameter, just as the number of particles N and its volume V. If we consider a set of systems which are all prepared with the ***same N, V and T,*** and with energies distributed according to the Boltzmann factor, we speak of ***a canonical, or (N, V, T) ensemble.***

13.3 System in the Canonical Ensemble

Let us consider a system in the canonical ensemble. The entropy of the system define in terms of the quantum density operator as

$$S = -k_B.[Tr(\rho \ln \rho)]$$

Writing

$$\rho = \sum |r\rangle P_r \langle r|$$

leads to the same expression as above

$$S = -k_B \sum P_r \, ln \, P_r$$

The basic postulate now is that, given expectation values for external parameters, the density matrix will assume a form which maximizes the entropy defined this way.

The (*NVE*) ensemble is the most natural one to define in classical or quantum mechanics:

(i) The number of degrees of freedom is well-defined (via the particle number N) and

(ii)The potential does not depend explicitly on time (the volume is fixed, i.e. the walls do not move).

(iii)The Hamiltonian is conserved and it can be identified with the energy.

Now suppose that there is a number M of states with the prescribed energy. We must find the distribution P_r which makes S stationary under the constraint that P_r is normalized. This is done using a Lagrange multiplier λ. We define

$$F = S - \lambda \sum_{r=1}^{M} P_r$$

and now require F to be stationary:

$$\frac{\partial F}{\partial P_r} = -k_B(1 + lnP_r) - \lambda$$

This leads to a family of solutions

$$P_r = \exp\left(-\frac{k_B + \lambda}{k_B}\right)$$

parametrised by λ. We must now adjust λ such as to satisfy the constraint that P_r be normalized. This then leads to

$$P_r = \frac{1}{M}$$

which is independent of r. We see that for the microcanonical ensemble, the distribution which maximizes the entropy is the one in which each state has the same probability of occurrence.

Instead of requiring that each of the parameters N, V or E be fixed, we may relax any of these conditions and require the expectation value to assume a certain value rather than the stronger condition that the parameter may only assume a certain value. We shall work this out for the energy. In the context of quantum mechanics,

this is a bit tricky as we must calculate the variation of an operator. However, if we assume that the density operator can be written in the form

$$\rho = \sum |r\rangle P_r \langle r|$$

with $|r\rangle$being eigenstates of the Hamiltonian, the solution of the problem is identical to the classical case.

We now have an additional constraint, that is,

$$\boxed{\langle E \rangle = \sum_r P_r E_r}$$

is given. Here E_r is the energy of the state r. We now have two Lagrange multipliers, one for the energy (which we call $k_B\beta$) and one (again λ) for the normalization:

$$F = S - \lambda \sum_r P_r - k_B \beta \sum_r P_r E_r$$

Following the same procedure as above, we find

$$P_r = \frac{1}{Q_\lambda} exp(-\beta\, E_r)$$

Q : the partition function – is defined in terms of the multiplier λ – it serves merely to normalize the probability distribution.

The Lagrange parameter β which we can identify with $1/k_B T$ serves as the parameter which can be tuned in order to adjust the expectation value of the energy to the required value. If we relax the particle number but fix its expectation value, we obtain

$$P_r = \frac{1}{Z_\lambda} exp(-\beta\, E_r - \sigma N)$$

where σ can be identified with $-\beta\mu$, μ is the chemical potential.

Let us analyze the canonical partition function a bit further. The expectation value of the energy can be determined as

$$\boxed{\langle E \rangle = -\frac{\partial}{\partial \beta} ln Q}$$

Using $P_r = exp(-\beta\, E_r)/Q$, we can write the entropy as

$$S = -k_B \sum_r P_r \ln P_r = -k_B \sum_r P_r[-\ln Q - \beta E_r] = k_B \ln Q - k_B \beta \frac{\partial}{\partial \beta} \ln Q$$

The transformation from S to $\ln Q$ which leads to this type of relation is known as the **Legendere transformation**.

Returning to the derivation of the canonical distribution function, we note that the function we have maximized can be written as

$$S = \lambda - T < E >$$

where we have used $\sum P_r = 1$ and $\sum_r P_r E_r = < E >$. Now we write this expression (disregarding the constant λ) as

$$-\frac{A}{T} = -\frac{E - TS}{T}$$

The quantity $\boxed{A = E - TS}$ is called ***the (Helmholtz) free energy***. We see that this quantity was minimized as a function of P_r. We have:

The Boltzmann distribution is the distribution which minimizes the Helmholtz free energy.

13.4 Physical Significance of the Various Statistical Quantities in the Canonical Ensemble

Energy defined as

$$\boxed{U = \langle E \rangle = \frac{\sum_r E_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}}$$

The denominator ensures proper normalization, in particular it ensures that the average value of 1 is equal to 1.

Looking at the above equation, we see that we can write U as

$$U = < E > = -\frac{\partial}{\partial \beta} \ln \sum_r e^{-\beta E_r}$$

It is useful to define $\boxed{Q_N = \sum_r e^{-\beta E_r}}$

Q is called the partition function.

Let us relate the quantities we have seen so far to thermodynamics. For a system at constant V, N and T, we know for the Helmholtz free energy

$A = E - TS$, that

$$dA = dU - TdS - SdT = -SdT - PdV + \mu dN:$$

From this, we have

$$\boxed{S = -\left(\frac{\partial A}{\partial T}\right)_{N,V}}$$

$$\boxed{P = -\left(\frac{\partial A}{\partial V}\right)_{N,T}}$$

$$\boxed{\mu = \left(\frac{\partial A}{\partial N}\right)_{T,V}}$$

From the first relation, we have:

$$U = A + TS = A - T\left(\frac{\partial A}{\partial T}\right)_{N,V} = T^2\left[\frac{\partial}{\partial T}\left(\frac{A}{T}\right)\right]_{N,V} = \left[\frac{\partial\left(\frac{A}{T}\right)}{\partial\left(\frac{1}{T}\right)}\right]_{N,V}$$

$$\boxed{U = A + TS = T^2\left[\frac{\partial}{\partial T}\left(\frac{A}{T}\right)\right]_{N,V} = \left[\frac{\partial\left(\frac{A}{T}\right)}{\partial\left(\frac{1}{T}\right)}\right]_{N,V}}$$

from which we can infer that

$$\boxed{A = -k_B \ln Q_N}$$

By taking the temperature derivative of U we obtain the expression for the specific heat:

$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = -T^2\left(\frac{\partial^2 A}{\partial T^2}\right)_{N,V}}$$

$$dA = -SdT - PdV + \mu dN$$

we see that if we keep the volume and the particle number constant, we have

$$dA = -PdV$$

that is, the change in free energy is completely determined by the work done by the system. The Hemholtz free energy represents the work which can be done by a closed, isothermal system.

We have seen that the probability P_r with which a configuration with energy E_r occurs, is given by the *Boltzmann factor*:

$$P_r = \frac{e^{-\frac{E_r}{k_B T}}}{Q_N}$$

The entropy can be calculated as

$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = \left(\frac{\partial k_B \ln Q_N}{\partial T}\right)_{N,V} = k_B \ln Q_N - \frac{U}{T}$$

We now replace U, which is the expectation value of E_r, by the expectation value of $-k_B T \ln Q_N P_r$

$$S = k_B \ln Q_N - < \ln Q_N P_r > = -k_B < \ln P_r > = -k_B \sum_r P_r \ln P_r$$

$$\boxed{S = -k_B \sum_r P_r \ln P_r}$$

From this relation, ***it follows that the entropy vanishes at zero temperature ('third law of thermodynamics').***

13.5 Self Learning Exercise -I

Short Answer Type Questions

Q.1 Why are the factors $\frac{1}{N!}$ and $1/h^{3N}$ introduced into the derivation of the partition function of the ideal classical gas?

Q.2 Explain canonical ensemble.

Q.3 Define Legendere transformation

Q.4 Explain a system in the canonical ensemble.

Q.5 What are the physical significance of the various statistical quantities in the canonical ensemble.

13.6 Partition Function

When one evaluating the sums over *states r*, we should not confuse those states with their energies. For a system with a strictly discrete spectrum, the

energies E_i might occur with a multiplicity (degeneracy) g_i. In that case, when we evaluate the sum over some energy dependent quantity, we have

$$\sum_r \rightarrow \sum_i g_i$$

In fact, the probability of having an energy E_i is given by

$$P_i = \frac{g_i e^{-\beta E_i}}{\sum_i g_i e^{-\beta E_i}}$$

In practice, the energy is usually continuous or almost continuous. In that case, g_i is replaced by the density of states $g(E)$. This quantity is defined as follows

Number of quantum states with energy between E and $E + dE = g(E)dE$.

$$P(E) = \frac{g(E)e^{-\beta E}}{\int_{-\infty}^{\infty} g(E)e^{-\beta E} dE}$$

13.7 Classical Systems

Now we evaluate expectation values for a system consisting of interacting point particles. In the micro canonical ensemble it was argued that the sum over the available quantum states can be replaced by

a sum over volume ω in phase space, provided we divide by the 'unit phase space volume' h^{3N} and by $N!$ in order to avoid over-counting of indistinguishable configurations obtained from each other by particle permutation. Therefore we have

$$Q_N = \frac{1}{h^{3N} N!} \int e^{-\beta H(q,p)} \, d^{3N} q \, d^{3N} p$$

where

$$H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(q_1, \ldots q_{3N})$$

For the ideal gas, $V \cong 0$. Note that the $\mathbf{p}_i$ are vectors in 3D.

The expression for Q_N looks quite complicated, but the integral over the momenta can be evaluated analytically.

$$\int e^{-\left(\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}\right)} d^{3N} p = \int e^{-\left(\beta \frac{p_1^2}{2m}\right)} d^{3N} p_1 \int e^{-\left(\beta \frac{p_2^2}{2m}\right)} d^{3N} p_2 \ldots \int e^{-\beta p_3^2/2m} d^{3N} p_3$$

The integral over one particle then factorizes into one over p_x, one over p_y and one over p_z. Now we use the Gaussian integral result:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{(\pi/\alpha)}$$

in order to obtain

$$Q_N = \frac{1}{N!}\left[\frac{(2\pi m k_B T)^{\frac{3}{2}}}{h^3}\right]^N \int e^{-\beta V} d^{3N} q$$

For an ideal gas, $V = 0$ and we can evaluate the remaining integral: it yields V^N .Therefore, the partition function of the ideal gas is found as

$$\boxed{Q_N = \frac{1}{N!}\left[\frac{V\left(2\pi m k_B T\right)^{\frac{3}{2}}}{h^3}\right]^N}$$

13.8 Energy Fluctuations in the Canonical Ensemble

In the canonical ensemble, the energy can take on any possible value between the ground state and infinity. The actual probability with which a particular value of the energy occurs is proportional to

$$P(E) \propto g(E)\, e^{-\frac{E}{k_B T}}$$

The prefactor $g(E)$ is the density of states. In general, we find that this quantity is a very strongly increasing function of the energy, whereas the Boltzmann function $e^{-\frac{E}{k_B T}}$ strongly *decreases* with energy. The result is that the probability distribution of the energy is very sharply peaked around its mean value $U = \langle E \rangle$. To show that the energy is indeed sharply peaked around U, we calculate the fluctuation. From statistics, we know that the width of the distribution is given by

$$(\Delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2$$

From

$$U = < E > = \frac{\sum_r E_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}$$

where, as usual, $\beta = 1/k_B T$, we see that

$$\frac{\partial U}{\partial \beta} = \left(\frac{\sum_r E_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} \right)^2 - \frac{\sum_r E_r^2 e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} = -(\Delta E)^2$$

The quantity $\partial U / \partial \beta$ is equal to

$$\frac{\partial U}{\partial \beta} = k_B T^2 \frac{\partial U}{\partial T} = k_B T^2 C_V$$

Realising that C_V is an extensive quantity, which scales linearly with N, we therefore have

$$\frac{\Delta E}{U} = \frac{\sqrt{k_B T^2 C_V}}{U} \sim 1/\sqrt{N}$$

In the thermodynamic limit, we see that the relative width becomes very small. Therefore, we see that the energy, which is allowed to vary at will, turns out to be almost constant. Therefore, we expect the physics of the system to be almost the same of that in the microcanonical ensemble (where the energy *is* actually constant).

This result is usually referred to as the 'equivalence of ensembles'.

13.9 The 'Equipartition' and the 'Virial' Theorems

The expectation value of the kinetic energy T is as follows.

$$< T > = \frac{\int \frac{p_i^2}{2m} \exp\left[-\frac{\left(\sum_i \frac{p_i^2}{2m} + V(R) \right)}{k_B T} \right] d^{3N} p d^{3N} R}{\int exp\left[-\frac{\left(\sum_i \frac{p_i^2}{2m} + V(R) \right)}{k_B T} \right] d^{3N} p d^{3N} R}$$

All sums over i run from 1 to N, R and p represent all positions and momenta.

Obviously, the contributions to the result from each momentum coordinate of each individual particle are identical, and they can be evaluated using the same

factorization which led to the evaluation of the partition function of the ideal gas (the integrals over the coordinates *R* cancel). We obtain

$$< T > = 3N \frac{\int \frac{p^2}{2m} exp\left[-\frac{p^2}{2mk_BT}\right] dp}{\int exp\left[-\frac{p^2}{2mk_BT}\right] dp} = \frac{3Nk_BT}{2}$$

This result is known as the ***equipartition theorem***.

It tells us that the kinetic energy for each degree of freedom is $k_BT/2$.

The second theorem gives us an expression for the pressure *P*. We know that

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T}$$

Now we replace *A* by $-k_BT \ln Q_N$

$$P = k_BT \frac{1}{Q_N} \frac{\partial Q_N}{\partial V}$$

First we realise that the integral over the momenta is volume-independent – therefore only the part

$$\widetilde{Q_N} = \int exp\left[-\frac{U(\vec{r}_1, \dots, \vec{r}_N)}{k_BT}\right] d^3R$$

is to be considered.

To evaluate the volume-dependence of this object, we write for the coordinates $\mathbf{r}_i$ of the particles:

$$\vec{r}_i = V^{\frac{1}{3}} \vec{s}_i$$

that is, the coordinates $\vec{s}_i$ are simply rescaled in such a way that they occupy a volume of the same shape as the $\vec{r}_i$, but everything is rescaled to a unit volume. Every configuration in a volume *V* has a one-to-one correspondence to a configuration of the $\vec{s}_i$. Therefore we can write

$$\int exp\left[-\frac{U(\vec{r}_1, \dots, \vec{r}_N)}{k_BT}\right] d^{3N}R = V^N \int exp\left[-\frac{U\left(V^{\frac{1}{3}} \vec{s}_1, \dots, V^{\frac{1}{3}} \vec{s}_N\right)}{k_BT}\right] d^{3N}S$$

where the prefactor arises because of the change of integration variables.

Now, the derivative with respect to *V* can be evaluated

$$\frac{\partial \widetilde{Q_N}}{\partial V} = NV^{N-1}\widetilde{Q_N} - \frac{V^{-\frac{2}{3}}}{3k_BT}\int \sum_i \vec{s}_i . \nabla_i U \, exp\left[-\frac{U\left(V^{\frac{1}{3}}\vec{s}_1, \ldots, V^{\frac{1}{3}}\vec{s}_N\right)}{k_BT}\right] d^{3N}S$$

Collecting all the terms we obtain

$$\frac{PV}{k_BTN} = 1 - \frac{1}{3Nk_BT}\left\langle \sum_{i=1}^{N} r_i . \frac{\partial U}{\partial r_i} \right\rangle$$

We see that for $U = 0$ we have $PV = Nk_BT$, which is well known for the ideal gas.

Very often interaction potentials are modeled as a sum over all particle pairs:

$$U(\vec{r}_1, \ldots, \vec{r}_N) = \sum_{i,j,j>i}^{N} u(|\vec{r}_i - \vec{r}_j|)$$

In that case, the rightmost term in the virial theorem can be rewritten as

$$\left\langle \sum_{i=1}^{N} r_i . \frac{\partial U}{\partial r_i} \right\rangle = \frac{N(N-1)}{2} < r\frac{\partial u(r)}{\partial r} > = \frac{N(N-1)}{2}\int_0^{\infty} r\frac{\partial u}{\partial r} g(|\vec{r}_1 - \vec{r}_2|) d^3r_1 d^3r_2$$

where we have introduced the pair correlation function, $g(r)$, which gives the probability of finding a particle pair at separation**.** The formal definition of $g(r)$ is

$$g(r) = \frac{V(\int \delta(|\vec{r}_1 - \vec{r}_2| - r) \exp(-\beta H)\, d^3r_1 \ldots d^3r_N)}{Q_N}$$

Because the particles are identical, we can take any pair instead of 1 and 2. For large separation r, $g(r)$ tends to 1. The virial theorem can be reformulated in terms of the pair correlation function.

$$\frac{PV}{Nk_BT} = 1 - \frac{2\pi}{3Nk_BT}\int_0^{\infty} g(r)\frac{\partial u(r)}{\partial r} r^3 dr$$

13.10 System of Harmonic Oscillators

Now we consider a classical system with an Hamiltonian given by

$$\mathrm{H(q,p)} = \frac{\sum_{i=1}^{N} \mathrm{p_i^2}}{2\mathrm{m}} + \frac{\mathrm{m}\omega^2}{2}\mathrm{q_i^2}.\mathrm{N}$$

For this system, the partition function can be evaluated analytically as the Hamiltonian is a quadratic function of both the momenta and the coordinates. The calculation therefore proceeds analogous to that for the ideal gas where the Hamiltonian is a quadratic function of the momenta only. The result for oscillator system is

$$\boxed{Q_N = \frac{1}{(\beta\hbar\omega)^N}}$$

where we have assumed that the oscillators are distinguishable. The free energy now follows as

$$A = -k_B T \ln Q_N = N k_B T \ln\left(\frac{\hbar\omega}{k_B T}\right)$$

From this we find

$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = N k_B \left[-ln\left(\frac{\hbar\omega}{k_B T}\right) + 1\right]$$

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T} = 0$$

$$\mu = \left(\frac{\partial A}{\partial N}\right)_{T,V} = k_B T\, ln\left(\frac{\hbar\omega}{k_B T}\right)$$

$$U = \left[\frac{\partial\left(\frac{A}{T}\right)}{\partial\left(\frac{1}{T}\right)}\right]_{N,V} = N k_B T$$

From the last equation, we find

$$C_V = N k_B = C_P$$

The fact that $U = N k_B T$ is in agreement with the equipartition theorem as the Hamiltonian has *two* independent quadratic terms (for *q and p*) instead of only one. It shows that for harmonic oscillators, the energy is equally divided over the potential and the kinetic energies.

Next we consider a collection of quantum harmonic oscillators in the canonical ensemble. This is simpler to evaluate than the classical case. The states for oscillator number *i* are labeled by n_i, hence

$$Q_N = \sum_{\{n_i\}} e^{-\beta\hbar\omega \sum_i \left(n_i + \frac{1}{2}\right)}$$

where $\sum_{\{n_i\}}$ denotes a sum over all possible values of all numbers n_i. This partition function factorizes in a way similar to the classical system, and we obtain

$$Q_N = \left(\sum_n e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)}\right)^N = \left(\frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\frac{\beta\hbar\omega}{2}}}\right)^N$$

From the partition function we obtain, similar to the classical case

$$A = N\ln[\frac{\hbar\omega}{2} + k_B T \ln(1 - e^{-\beta\hbar\omega})]$$

And, from this,

$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = Nk_B\left[\frac{\beta\hbar\omega}{(e^{-\beta\hbar\omega} - 1)} - ln(1 - e^{-\beta\hbar\omega})\right]$$

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T} = 0$$

$$\mu = \left(\frac{\partial A}{\partial N}\right)_{T,V} = \frac{A}{N}$$

$$U = \left[\frac{\partial\left(\frac{A}{T}\right)}{\partial\left(\frac{1}{T}\right)}\right]_{N,V} = N\left[\frac{\hbar\omega}{2} + \frac{\hbar\omega}{(e^{\beta\hbar\omega} - 1)}\right]$$

And, finally

$$C_V = C_P = Nk_B(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

Interestingly, the quantum harmonic oscillator does not obey equipartition: we see that only the first term in the expression for the energy is in accordance with that theorem – the second term gives a positive deviation from the equipartition result.

13.11 The Statistics of Paramagnetism

Consider a system consisting of a set of magnetic moments. Each moment interacts with a magnetic field $\vec{H}$, but the interaction between the moments is neglected. In that case we can consider again a system of only one magnetic moment and construct the partition function for *N* moments by raising that for a single moment to the *N*-th power.

The interaction Hamiltonian is given by $\mathcal{H} = -\vec{\mu}.\vec{H}$

Note the difference between the Hamiltonian $\mathcal{H}$ and the field $\vec{H}$. Without loss of generality we can take $\vec{H}$ along the *z*-direction so that

$$\mathcal{H} = -\mu H cos v$$

where v is the angle between the moment and the *z*-axis.

The partition function can now be evaluated:

$$Q_1 = \int e^{\beta\mu H\cos v}\, sinv\, dv\, d\varphi = \frac{4\pi \sinh(\beta\mu H)}{\beta\mu H}$$

We can also calculate the average value of the magnetic moment

$$\bar{\mu}_z = \frac{\int_0^{2\pi}\int_0^{\pi} \mu\, e^{\beta\mu H\cos v}\cos v\, sinv\, dv\, d\varphi}{\int_0^{2\pi}\int_0^{\pi} e^{\beta\mu H\cos v}\, sinv\, dv\, d\varphi} = \mu\left[\coth(\beta\mu H) - \frac{1}{\beta\mu H}\right] = \mu L(\beta\mu H)$$

where $L(x)$ is the Langevin function.

For high temperatures, that is, for small values of x, the Langevin function behaves as $L(x) \sim 1/(3x)$, so we have

$$M = \frac{\mu^2}{3k_B T} H$$

The magnetic susceptibility is defined as

$$\chi = \partial M/\partial H$$

therefore has the form

$$\chi = \frac{C}{T}$$

where C is the so-called Curie constant. This relation is known as the ***Curie law of paramagnetism.***

13.12 Negative Temperature

The case of paramagnetic $s = 1/2$ spins is the easiest example of a quantum magnetic system. In that case, the spins assume values either $\hbar/2$ or $-\hbar/2$ when they are measured along an arbitrary axis. If we apply a magnetic field $\vec{H}$, there are therefore two possible values of the energy for these two orientations ; we call these energies ε and $-\varepsilon$. Therefore we immediately find that the partition sum is given as:

$$Q_N(\beta) = \left(e^{-\beta\epsilon} + e^{\beta\varepsilon}\right)^N = [2\cosh\beta\varepsilon]^N$$

The fact that the term in brackets can simply be raised to the N^{th} power is a result of the fact that the spins do not interact mutually.

The thermodynamic properties from the partition function

$$A = -Nk_B T \ln[2\cosh(\varepsilon/k_B T)]$$

$$S = -\left(\frac{\partial A}{\partial T}\right)_{N,V} = Nk_B\{\ln[2\cosh(\beta\varepsilon) - \beta\varepsilon\tanh(\beta\varepsilon)]\}$$

$$U = A + TS = -N\varepsilon \tanh \beta\varepsilon$$

$$M = -\left(\frac{\partial A}{\partial H}\right)_T = N\mu_B \tanh \beta\varepsilon$$

where μ_B is the Bohr magneton: the coupling constant between the spin and the external field, i.e.

$$\epsilon = \mu_B H$$

Finally we have

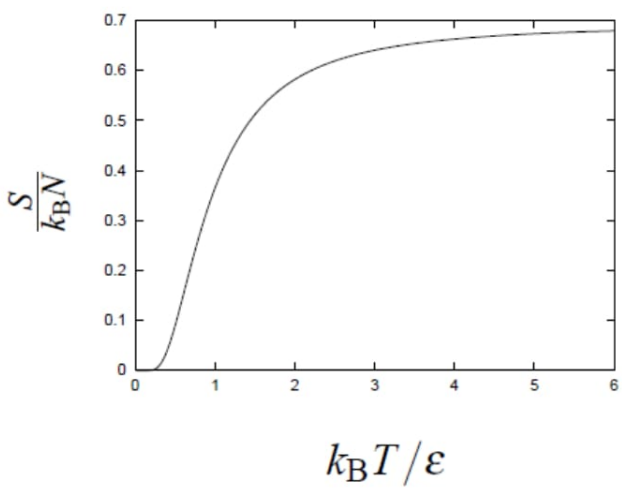
$$C_H = \frac{\partial U}{\partial T}_H = N k_B (\beta\epsilon)^2 / \cosh^2(\beta\varepsilon)$$

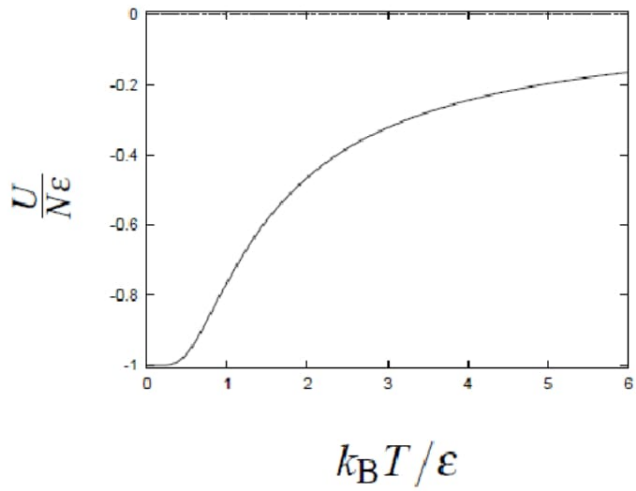
We see that $U = -MH$, as could be expected. In the next few figures we show the temperature dependence of S, U, M and C_H. These graphs show several interesting features.

(i)The temperature dependence of Entropy: The entropy vanishes for small temperature as it should, this shows that for low temperatures nearly all spins are in line with the field, so that the entropy is low. Also, the energy per spin is about −ε. When we increase the temperature, more and more spins flip over and the entropy and energy increase. There will be a particularly strong increase in the entropy near $k_B T = \varepsilon$ as in that region the thermal energy is sufficiently strong for flipping the spins over. For high temperatures the spins assume more or less random orientations, and the entropy will approach a constant.

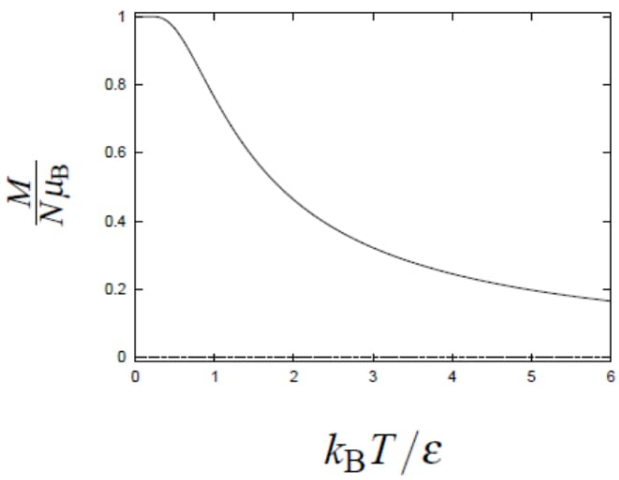
(ii) The graph of the magnetization is also easily explained now.

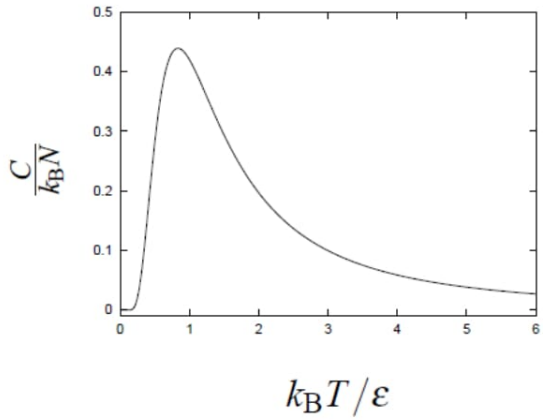
(iii) The specific heat shows a maximum near $k_B T = \varepsilon$ for the reason just explained.





1. **The temperature dependence of Energy** A striking feature of the energy graph is that it does not approach its maximum value, which is reached when all spins would be antiparallel to the field. In fact, when the energy is positive, the entropy will decrease with energy. This can be used in an experimental technique called magnetic cooling. In this technique, a strong magnetic field is suddenly reversed in order to bring the spins in a configuration where the majority is antiparallel to the field. In that case, the temperature is negative, as the entropy decreases with energy and $1/\mathrm{T} = \partial \mathrm{S}/\partial \mathrm{E}$. This is not in contradiction with the laws of thermodynamics, as the system is far from equilibrium. In order to reach equilibrium, the temperature will return to positive values, and it therefore has to pass through absolute zero. The system is therefore extremely cold for some time.





13.13 Self Learning Exercise II

Short Answer Type Questions

Q.1 Show that for high temperatures, i.e. , for small values of x, the Langevin function behaves as $L(x) \sim 1/(3x)$.

Q.2 Plot Langevin function L(x) as a function of x.

Q.3 State Curie law of paramagnetism.

Q.4 Define Bohr magneton.

Long Answer Type Questions

Q.5 Explain the phenomena of magnetic cooling.

13.14 Summary

In this unit we discussed equilibrium between a system and a heat reservoir, canonical ensemble, physical significance of the various statistical quantities in the canonical ensemble, partition function, classical system, energy fluctuations in the canonical ensemble, 'equipartition' and 'virial' theorem, system of harmonic oscillators, statistics of paramagnetism and negative temperatures.

13.15 Glossary

Partition function: A function determined by the probability distribution (over phase space in the classical treatment; over quantum states in the quantum treatment) describing a thermally equilibrated system; many thermodynamic quantities can be expressed in terms of the partition function and its derivatives.

***Heat Reservoir*:** Surroundings at a certain temperature which are large enough to absorb heat from, or donate heat to, the system without appreciable change of temperature. Also heat bath

***Reversible*:** A reversible process is one which would change direction with an infinitesimal change in external conditions. For a process to be reversible it must be frictionless and quasistatic so that no energy is dissipated and the system is always only infinitesimally removed from equilibrium. Because a reversible process passes through a series of quasi-equilibrium states it can be represented as a solid line on a plot of one state variable against another.

Surroundings: That part of an experimental set up, including the ambient air, which exchanges heat with, or does work on, the system.

Universe: A deliberately grandiose term for the entire experimental set-up, comprising the system and the surroundings. Usually encountered in the phrase ``the entropy change of the universe" which of course cannot be negative, though that of the system or surroundings alone may be. It should not be confused with the cosmological universe.

***Internal energy U*:** is the total energy of the system. It contains the translational, rotational, vibrational, electronic, and nuclear energies and the energies due to intermolecular interactions. Its absolute value is unknown, its change is defined by the first law of thermodynamics. It is a state function and an extensive quantity.

State function: It is a property that is determined by the state of the system. The change in the state function is path independent and defined by the properties in the initial and the final state only.

13.16 Answer to Self Learning Exercises

Answer to Self Learning Exercise- I

Ans.1: The factor $\frac{1}{N!}$ is needed to account for the fact that when an integration is carried out over all phase space for N particles, all permutations of the particle identities is included. For indentical particles this must be removed. The factor $\frac{1}{h^{3N}}$takes account of the Heisenberg uncertainty principle which states that the smallest phase space volume that makes sense is $\left(\frac{\hbar}{2}\right)^3$. The fact that it is

$\frac{1}{h^3}$ instead of $1/\left(\frac{\hbar}{2}\right)^3$ for each particle is to reproduce the high temperature behavior of quantum gases.

Ans.2: It is an ensemble in which the macrostate of the systems is defined through the parameters *N*,*V*, and *T*.

Ans.3: The transformation from *S* to *lnQ* which leads to below type of relation is known as the **Legendere transformation**.

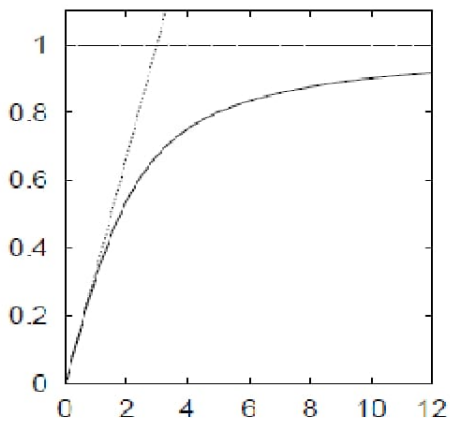
$$S = -k_B \sum_r P_r \ln P_r = -k_B \sum_r P_r[-\ln Q - \beta E_r] = k_B \ln Q - k_B \beta \frac{\partial}{\partial \beta} \ln Q$$

Ans.4: Section 13.3

Ans.5: Section 13.4

Answer to Self Learning Exercise -II

Ans.1,2:



Ans.3: $\chi = \frac{C}{T}$

where *C* is the so-called Curie constant. This relation is known as the *Curie law* of paramagnetism.

Ans.4: Bohr magneton μ_B define as the coupling constant between the spin and the external field, i.e. $\epsilon = \mu_B H$

Ans.5: In this technique, a strong magnetic field is suddenly reversed in order to bring the spins in a configuration where the majority is antiparallel to the field. In that case, the temperature is negative, as the entropy decreases with energy and $1/T = \partial S/\partial E$. This is not in contradiction with the laws of thermodynamics, as the system is far from equilibrium. In order to reach equilibrium, the temperature will

return to positive values, and it therefore has to pass through absolute zero. The system is therefore extremely cold for some time.

13.17 Exercise

Short Answer Type Questions

Q.1 Show the temperature dependence of S, U, M and C_H

Long Answer Type Questions

Q.2 Prove that the quantum harmonic oscillator does not obey equipartition theorem while classical harmonic oscillator obeys equipartition theorem.

Q.3 Paramagnets and also the Ising model in one dimension exhibit a peak in their specific heat, with the low temperature behavior being an approach to zero exponentially and at high temperature an approach to zero as $\frac{1}{T^2}$. Why is there a peak in the specific heat in these models. What can't we use the rule $\frac{k_B T}{2}$ per degree of freedom to find the specific heat?

Q.4 Explain the physical origins of the paramagnetic and diamagnetic contributions to the magnetization of the free electron gas.

References and Suggested Readings

1. L. D. Landau and E. M. Lifshitz, Statistical Physics, 3rd Edition, Butterworth-Heinmann, 1980.
2. H. B. Callen, Thermodynamics and an Introduction to Thermo-statistics, 2nd Edition, Wiley, 1985.
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UNIT-14
The Grand Canonical Ensemble

Structure of the Unit

14.0 Objectives

14.1 Introduction

14.2 Equilibrium between a System and Reservoir

14.3 The grand Canonical Ensemble

14.4 Physical significance of the various Statistical quantities

14.5 Self Learning Exercise -I

14.6 Illustrative Examples

14.7 Density and energy fluctuations in the grand canonical ensemble

14.8 Comparisons between microcanonical, canonical and grand canonical ensembles

14.9 Self Learning Exercise- II

14.10 Summary

14.11 Glossary

14.12 Answer to Self Learning Exercises

14.13 Exercise

References and suggested Readings

14.0 Objectives

After interacting with the material presented here students will be able to understand

1. The grand canonical ensemble
2. Physical significance of the various statistical quantities,
3. Density and energy fluctuations in the grand canonical ensemble

14.1 Introduction

In statistical mechanics, a grand canonical ensemble is the statistical ensemble that is used to represent the possible states of a mechanical system of particles that is being maintained in thermodynamic equilibrium (thermal and chemical) with a reservoir. The system is said to be open in the sense that the system can exchange energy and particles with a reservoir, so that various possible states of the system can differ in both their total energy and total number of particles. The system's volume, shape, and other external coordinates are kept the same in all possible states of the system.

The thermodynamic variables of the grand canonical ensemble are chemical potential (μ) and absolute temperature(T). The ensemble is also dependent on mechanical variables such as volume (V) which influence the nature of the system's internal states. This ensemble is therefore sometimes called the μVT ensemble, as each of these three quantities are constants of the ensemble.

14.2 Equilibrium between a System and Reservoir

Let us consider a large, isolated system in which we define a subsystem, which can exchange not only energy, but also particles with the remainder of the large system (the remainder is again called a bath). (Shown in figure). Now we consider a state s of the subsystem consisting of N_r particles and an energy E_s. Just as in the derivation of the canonical ensemble, we note that the probability of occurrence of this state is proportional to the number of possible states of the bath

$$P_{r,s} \propto \Omega(E - E_s, N - N_r)$$

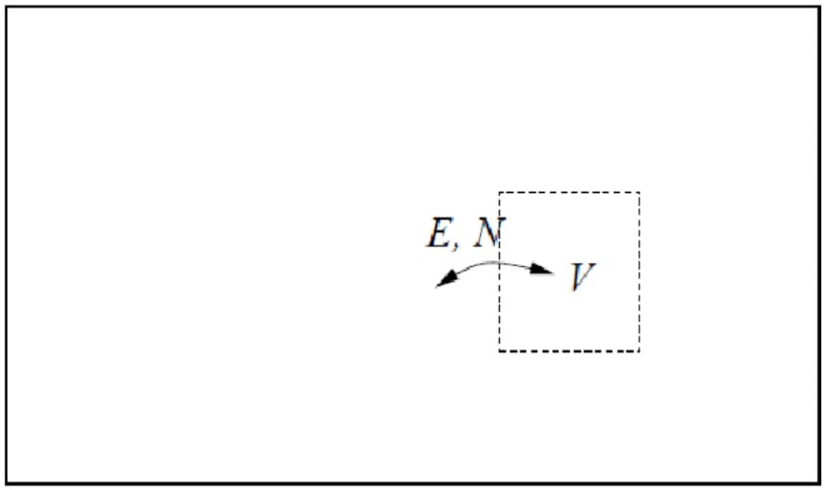
Writing $\Omega = \exp(S/k_B)$ and realizing that

$$\frac{\partial S}{\partial E} = \frac{1}{T}$$

$$\frac{\partial S}{\partial N} = -\frac{\mu}{T}$$

we obtain

$$P_{r,s} \propto e^{\frac{S(E-E_s,N-N_r)}{k_B}} \propto e^{-\beta E_s + \beta \mu N_r}$$



We see that the probability distribution is that of the canonical ensemble multiplied by an extra factor $\exp(\beta\mu N)$ and summed over N. The required normalization factor is

$$\sum_{N=0}^{\infty} e^{\beta\mu N} \sum_{s} E_s e^{-\beta E_s} \equiv Z$$

The quantity Z is called the ***grand canonical or grand partition function.***

14.3 The Grand Canonical Ensemble

Using the principle of maximum entropy, we can derive the probability for the grand canonical ensemble. We do this by requiring the expectation values of E and N are given.

Hence we must maximize the entropy

$$S = -k_B \sum_{N} \sum_{r} P_r(N) \ln p_r(N)$$

under the condition that

$$\sum_{N} \sum_{r} P_r(N) E_r(N) = < E > = U$$

is given and that

$$\sum_{N} N \sum_{r} P_r(N) = < N >$$

This then leads to a Lagrange function

$$F = S - \lambda \sum_N \sum_r P_r(N) - k_B\beta \sum_r P_r(N)E_r(N) - k_B\beta\mu \sum_N N \sum_r P_r(N)$$

Taking the derivative with respect to $p_r(N)$ leads to

$$-k_B \ln p_r\,(N) - k_B - \lambda - k_B\beta\, E_r(N) + k_B\beta\mu N = 0$$

leading to the distribution

$$p_r(N) = \frac{e^{-\beta E_r(N)+\beta\mu N}}{\sum_N \sum_r e^{-\beta E_r(N)+\beta\mu N}}$$

The denominator in this expression is called the grand canonical partition function

$$\boxed{Z = \sum_N \sum_r e^{-\beta E_r(N)+\beta\mu N}}$$

14.4 Physical Significance of the Various Statistical

The grand partition function can be written as

$$Z = \sum_{N=0}^{\infty} e^{\beta\mu N}\, Q_N(N,V,T)$$

where $Q_N(N,V,T)$ is the canonical partition function, which is related to the Helmholtz free energy A as

$$Q_N = e^{-\frac{A}{k_B T}}$$

The grand canoncial partition function can thus be written as

$$Z = \sum_{N=0}^{\infty} e^{\beta(\mu N - A)}$$

Just as in the case of the energy in the canonical ensemble, the summand $e^{\beta(\mu N-A)}$ will be very sharply peaked near the equilibrium value $\bar{N}$ of N, so that we may replace the sum by the summand at its peak value. In this way we find

$$k_B T\, lnZ = \mu\bar{N} - A$$
$$= \mu\bar{N} - U + TS$$

Using the Euler relation from thermodynamics,

$$U = ST - PV + \mu N$$

we find

$$k_B T\, lnZ \;=\; PV \equiv\; k_B T_q$$

Note that we have been a bit sloppy in replacing the sum over *N* by its maximum value – we should have included a width here. However, this only leads to an additive constant in the relation between $\mu\bar{N} - A$ and $k_B T\, lnZ$, which can be fixed by noting that for $\bar{N} = 0$, the right hand side should vanish, and the result obtained turns out to be correct.

Let us now calculate the average value of *N* using the density function:

$$N \;= \frac{\sum_{N=0}^{\infty} N e^{\beta(\mu N - A)}}{\sum_{N=0}^{\infty} e^{\beta(\mu N - A)}} = \; k_B T \left(\frac{\partial q(\mu, V, T)}{\partial \mu}\right)_{V,T}$$

Instead of the chemical potential μ, often the parameter $z \;=\; exp(\beta\mu)$ is used. The energy can be obtained as

$$\bar{U} \;=\; k_B T^2 \left(\frac{\partial q(z, V, T)}{\partial \mu}\right)_{z,T}$$

Note that in the derivative with respect to *T*, $z \;=\; exp\left(\frac{\mu}{k_B T}\right)$ is kept constant (though it depends on *T*).

The relations with thermodynamic quantities can most easily be formulated as

$$N \;= \left(\frac{\partial k_B T lnZ}{\partial \mu}\right)_{V,T}$$

$$P \;= \left(\frac{\partial k_B T lnZ}{\partial V}\right)_{\mu,T}$$

$$S \;= \left(\frac{\partial k_B T lnZ}{\partial T}\right)_{\mu,V}$$

14.5 Self Learning Exercise-I

Section A : Very Short Answer Type Questions

Q.1 Write down the grand canonical partition function.

Q.2 Define grand canonical ensemble.

Section B : Short Answer Type Questions

Q.3 Write down the thermodynamic variables of the grand canonical ensemble.

Q.4 Explain physical significance of the various statistical quantities.

14.6 Illustrative Examples

We first calculate the grand canonical partition function of the ideal gas. We start from the canonical partition function, which has the form

$$Q_N(N,V,T) = \frac{V^N}{N!}\left(\frac{\sqrt{2\pi m k_B T}}{h}\right)^{3N}$$

Now

$$Z = \sum_{N=0}^{\infty} e^{\beta\mu N}\frac{V^N}{N!}\left(\frac{\sqrt{2\pi m k_B T}}{h}\right)^{3N}\sum_{N=0}^{\infty}\frac{\xi^N}{N!} = exp(\xi)$$

with

$$\xi = Vz\left(\frac{\sqrt{2\pi m k_B T}}{h}\right)^{3} = Vz\Lambda^{-3}$$

The quantity $\Lambda = \left(\frac{\sqrt{2\pi m k_B T}}{h}\right)^{-1}$ is called the *de Broglie wavelength* – it depends on T only. From this expression for the grand canonical partition function, the thermodynamic quantities can easily be evaluated using the relations given in the previous section.

$$P = zk_BT/\Lambda^3$$

$$N = \frac{zV}{\Lambda^3}$$

$$U = zVk_BT^2\frac{d\Lambda^{-3}}{dT}$$

$$S = Nk_B\, ln\, z + zVk_B\left[T\frac{d\Lambda^{-3}}{dT} + \Lambda^{-3}\right]$$

The first two of these relations can be combined into the well-known equation of state

$$PV = Nk_BT$$

Interestingly, this relation does not depend on Λ, so it holds for other, *uncoupled* systems too, such as a system consisting of indistinguishable harmonic oscillators.

In a solid, consisting of atoms vibrating around their equilibrium position, the oscillators are *localized*. This has two important implications: first of all, they are distinguishable, and, secondly, the partition function of one such oscillator does not depend on the volume. This leads to the following form of the partition function:

$$Q_N(N,V,T) = \left(Q_1(T)\right)^N$$

Writing

$$Q_1(T) \equiv \varphi\,(T)$$

this leads straightfordly to

$$Z = \sum_N z^N[\varphi(T)]^N = \frac{1}{1-z\varphi(T)}$$

We see that $z\varphi(T)$ must be smaller than 1 in order for this sum to converge. From the partition sum the thermodynamic quantities can again be derived:

$$N = \frac{z\varphi\,(T)}{1-z\varphi\,(T)}$$

$$U = \frac{zk_BT^2\varphi'\,(T)}{1-z\varphi\,(T)}$$

$$A = Nk_BT\,ln\,z + k_BT\,ln\,[1-z\varphi\,(T)]$$

$$S = -Nk_B\,ln\,z - k_B\,ln\,[1-z\varphi\,(T)] + \frac{zk_BT\varphi'\,(T)}{1-z\varphi\,(T)}$$

From the second of these equations, we see that

$$z\varphi(T) = \frac{N}{1+N} \approx 1 - \frac{1}{N}$$

for large *N*. This renders the other relations a bit simpler

$$\frac{U}{N} = k_BT^2\varphi'\,(T)/\varphi\,(T)$$

$$\frac{A}{N} = -k_BT\,ln\varphi(T);$$

$$\frac{S}{Nk_B} = ln\varphi(T) + T\varphi'\,(T)/\varphi(T)$$

For quantum harmonic oscillators, we have

$$\varphi(T) = \sum_n \frac{e^{-\frac{\beta\hbar\omega}{2}}}{(1-e^{-\beta\hbar\omega})} = \frac{1}{2sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

For classical harmonic oscillators we have, on the other hand,

$$\varphi = (\beta\hbar\omega)^{-1}$$

We now use these results in order to analyze the solid-vapor equilibrium.

Solid and vapor are in equilibrium when their chemical potentials are equal. For the gas, we have

$$z_g = N_g\Lambda^3/V_g$$

with Λ the de Broglie wavelength $\Lambda = \left(\frac{\sqrt{2\pi m k_B T}}{h}\right)^{-1}$

For the solid, which we describe a system composed of many independent oscillators, we have

$$z_s = \frac{1}{\varphi(T)}$$

The equilibrium is achieved for a gas density

$$N_g/V_g = 1/\Lambda^3\varphi(T)$$

For low vapour density and high enough temperature, we therefore find

$$P = \frac{N_g}{V_g}k_BT = k_BT/(\Lambda^3\varphi(T))$$

which follows immediately from the ideal gas equation of state.

For 3D harmonic oscillators, we have

$$\varphi(T) = \left[2\sinh\left(\frac{\hbar\omega}{2k_BT}\right)\right]^{-3}$$

We have however not taken into account the fact that the energy at the equilibrium point of the harmonic oscillator describing an atom is lower than the energy of a gas atom: after all, the atom is bound to the solid, and we need a certain amount of energy to remove it from there and move it to the gas.

As a result, we must include a factor $\exp(\beta\varepsilon)$ in the product $\Lambda^3\varphi(T)$. We then arrive at an expression for the vapor pressure

$$P = \frac{N_g}{V_g} k_B T = k_B T \left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}} \left[2\, sinh\left(\frac{\hbar\omega}{2k_B T}\right)\right]^3 e^{-\beta\varepsilon}$$

We see that two parameters enter this equation: the energy difference ε and the frequency ω. These two parameters precisely determine shape and offset of the parabola's defining the energy felt by an atom in the solid.

14.7 Density and Energy Fluctuations in the Grand Canonical

Average number of particles

$$< N > = k_B T \frac{1}{z}\frac{\partial z}{\partial \mu} = k_B T \frac{\partial \ln z}{\partial \mu} = z\frac{\partial(\ln z)}{\partial z}$$

$$< N^2 > = (k_B T)^2 \frac{1}{z}\frac{\partial^2 \ln z}{\partial \mu^2}$$

$$\frac{\partial < N >}{\partial \mu} = \frac{1}{k_B T}\left(< N^2 > - < N >^2\right) = \frac{(\Delta N)^2}{k_B T}$$

Particle density

$$\rho = \frac{< N >}{V}, < N > = \rho V$$

$$\frac{V\partial\rho}{\partial\mu} = \frac{(\Delta N)^2}{k_B T}$$

$$(\Delta N)^2 = k_B T \frac{V\partial\rho}{\partial\mu}$$

$$(\Delta N) = \sqrt{(k_B T \frac{V\partial\rho}{\partial\mu})}$$

$$(\Delta N)/< N > = \sqrt{(k_B T \frac{V\partial\rho}{\partial\mu})}\frac{}{\rho V} \propto \frac{1}{\sqrt{V}} \to 0 \;\; (as\, V \to \infty)$$

Energy Fluctuation

The probability density of the ensemble as

$$P = z^{-1}\exp(-\beta E - \alpha N)$$

$$\beta = \frac{1}{k_B T}$$

$$\alpha = -\frac{\mu}{T}$$

Now the mean energy is

$$< E > = \frac{1}{z}\sum_{n=0}^{\infty}\int E\, exp(-\beta E - \alpha N)\, dV$$

Where

$$dV = d^N p\, d^N q\, /(\hbar^{3N} N!)$$

Differentiating mean energy with respect to the inverse temperature, we obtain

$$\frac{\partial}{\partial\beta} < E > = \frac{\partial}{\partial\beta}\frac{1}{z}\sum_{n=0}^{\infty}\int E\, exp(-\beta E - \alpha N)\, dV - < E^2 >$$

but using the definition of the partition function z we easily obtain

$$\frac{\partial}{\partial\beta}\frac{1}{z} = z^{-1} < E >$$

and so

$$\frac{\partial}{\partial\beta} < E > = < E >^2 - < E^2 \geq -variance\ E$$

in an entirely analogous fashion we can obtain

$$\partial/\partial\alpha < N > = < N >^2 - < N^2 \geq -variance\ N$$

It is of interest to consider what happens to fluctuations as the mean number of molecules increases i.e. as the thermodynamical limit is approached.

The mean energy per molecule

$$\varepsilon \equiv < E > /N$$

If ε is held fixed and the number of molecules increased then we simply

obtain a larger version of the original system.

$$\Delta_E \equiv \frac{sd(E)}{< E >} = \frac{1}{\sqrt{N\varepsilon}}\left(-\frac{\partial \varepsilon}{\partial \beta}\right)^{\frac{1}{2}}$$

which shows that as the size of the system increases the ratio of fluctuations of energy to system mean energy drops off as the inverse of the square root of the mean number of molecules.

14.8 Comparisons between Microcanonical, Canonical and Grand Canonical Ensembles

The **microcanonical** ensemble applies to isolated systems of many particles that do not exchange energy or particles with their environment. The fundamental assumption of statistical mechanics says that any microscopic configuration of such a system that respects global conservation laws (e.g., conservation of total energy U or particle number N) becomes equally likely after sufficient time. Thus, time averages of physical quantities become equal to averages over a statistical ensemble that weighs all relevant microscopic configurations equally. This is the microcanonical ensemble. The fundamental assumption does not always hold (e.g., in 'integrable' systems with a large number of conserved quantities), but it does apply to a very broad class of physical systems, underpinning the success of equilibrium statistical mechanics.

The **canonical** ensemble applies to a system coupled to a large environment with which it can exchange energy (i.e., an energy "reservoir"). Suppose that we can describe the whole system + reservoir by a microcanonical ensemble. Then, the probability of the system being in a particular configuration of energy E is simply proportional to the number of ways of depositing the remaining energy U-E in the reservoir. The probabilities implied by this procedure define the canonical ensemble. This construction also motivates the definition of temperature as the derivative of the number of configurations available to the reservoir as a function of its energy content. Note that the description of the canonical ensemble is very appropriate to real world materials, for instance, that absorb/emit radiation to/from their environment.

The grand canonical ensemble applies to a system coupled to a large environment with which it can exchange energy and particles (i.e., a particle and energy reservoir). The construction of this ensemble is completely analogous to the canonical ensemble: we apply the microcanonical ensemble to the system + reservoir and then consider the probability of a particular configuration of the system. This construction motivates the definition of the chemical potential.

Variable quantity	**Partition function**	**Characteri -stic function**	**Ensemble**	**Thermodynamic Differential from statistical mechanics**
none	$kTln\ Z(U,V,N)$	*TS*	Microcan onical	$dS = \frac{dU}{T} + \frac{P}{T}dV - \frac{\mu}{T}dN$
E_j	$-kTln\ Z(T,V,N$	*TS−U=A*	canonical	$dA = -SdT - PdV + \mu dN$
E_j, N_j	$kTln\ Z(T,V,\mu)$	TS−U+μN =PV	Grand-canonical	$d(PV) = -SdT + pdV + Nd\mu$

14.9 Self Learning Exercise-II

Section A : Very Short Answer Type Questions

Q.1 Define de Broglie wavelength.

Q.2 Compare canonical and grand canonical ensembles.

Section B : Short Answer Type Questions

Q.3 Calculate the thermodynamic quantities.

Q.4 Prove that for the quantum harmonic oscillators

$$\varphi(T) = \sum_n e^{-\frac{\beta\hbar\omega}{2}}/(1-e^{-\beta\hbar\omega}) = \frac{1}{2sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

And for classical harmonic oscillators

$$\varphi = (\beta\hbar\omega)^{-1}$$

Q.5 Derive an expression for the vapor pressure.

14.10 Summary

In this unit we discussed

- The grand canonical ensemble
- Equilibrium between a system and reservoir
- Physical significance of the various statistical quantities and examples
- Density and energy fluctuations in the grand canonical ensemble
- Comparisons between microcanonical, canonical and grand canonical ensembles

14.11 Glossary

System: That part of an experimental system in which we are primarily interested.

Internal energy U : It is the total energy of the system. It contains the translational, rotational, vibrational, electronic, and nuclear energies and the energies due to intermolecular interactions. Its absolute value is unknown, its change is defined by the first law of thermodynamics. It is a state function and an extensive quantity.

Macroscopic : Pertaining to aspects of a system which can be measured classically, such as temperature, pressure etc; containing very large numbers of atoms

Microscopic: Pertaining to the underlying quantum state of a system

Enthalpy H : H=U+PV, where U is the internal energy, P pressure and V volume. Its change gives the heat at constant pressure when there is no other work.

Entropy: (S, inJ/K) is a thermodynamic quantity that expresses the degree of disorder or randomness in a system at the molecular level.

Helmholtz energy (A): defined as A=U−TS, where U is the internal energy, T is the thermodynamic temperature and S is the entropy. The change in Helmholtz energy at constant volume and temperature gives the maximal work available. In a

closed system at constant volume and temperature the Helmholtz energy decreases during a spontaneous process.

Gibbs energy (G, in J): defined as G=H−TS, where H denotes enthalpy, T the thermodynamic temperature and S the entropy. The change in Gibbs energy at constant pressure and temperature gives the maximal work available. In a closed system at constant pressure and temperature the Gibbs energy decreases during a spontaneous process.

14.12 Answer to Self Learning Exercises

Answer to Self Learning Exercise- I

Ans.1:

$$Z = \sum_{N} \sum_{r} e^{-\beta E_r(N) + \beta \mu N}$$

Ans.2: A grand canonical ensemble is the statistical ensemble that is used to represent the possible states of a mechanical system of particles that is being maintained in thermodynamic equilibrium (thermal and chemical) with a reservoir.

Ans.3: Thermodynamic variables of the grand canonical ensemble are chemical potential (μ) and absolute temperature(T).

Ans.4: Section 14.5

Answer to Self Learning Exercise- II

Ans.1: $\Lambda = \left(\frac{\sqrt{2\pi m k_{BT}}}{h}\right)^{-1}$ is called the *de Broglie wavelength.*

Ans.3:

$$P = z k_B T / \Lambda^3$$

$$N = \frac{zV}{\Lambda^3}$$

$$U = zV k_B T^2 \frac{d\Lambda^{-3}}{dT}$$

$$S = N k_B \ln z + z V k_B \left[T \frac{d\Lambda^{-3}}{dT} + \Lambda^{-3} \right]$$

Ans. 4,5: Section 14.6

14.13 Exercise

Short Answer Type Questions

Q.1 Find Z as a function of T, V, μ.

Q.2 Find the grand potential from $\Omega = kT \ln Z$.

Q.3 Find the entropy of the system from

$$S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu}$$

and the number of particles from

$$N =< N >= -\left(\frac{\partial \Omega}{\partial \mu}\right)_{V,T}$$

Long Answer Type Questions

Q.4 Use

$$P = -\left(\frac{\partial \Omega}{\partial V}\right)_{\mu,T}$$

to find the equation of state.

Q.5 Find any useful thermodynamic potential from

$F = \Omega + \mu N$

$E = F + TS = \Omega + \mu N + TS$

$G = E + PV - TS = F + PV$

$H = E + PV$

Q.6 Does the Grand Canonical Ensemble allow for exchange of particles or not?

Q.7 What are the macroscopic conditions defining the grand canonical ensemble? What is needed to make it equivalent to the canonical and microcanonical ensembles?

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1. L. D. Landau and E. M. Lifshitz, Statistical Physics, 3rd Edition, Butterworth

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UNIT-15
Formulation of Quantum Statistics

Structure of the Unit

15.0 Objectives

15.1 Introduction

15.2 Statistics of the various ensembles

15.3 Electron in a magnetic field

15.4 Self learning exercise I

15.5 Free particle in a box

15.6 Linear oscillator

15.7 Systems of indistinguishable particles

15.8 The density matrix and the partition function of a system of free particles

15.9 Self learning exercise II

15.10 Summary

15.11 Glossary

15.12 Answer to self learning exercise

15.13 Exercise

References and Suggested Readings

15.0 Objectives

After interacting with the material presented here students will be able to understand

- The concept of quantum statistical mechanics
- Density matrix and density operator
- Various examples of quantum statistics as
- An electron in a magnetic field
- A free particle in a box

- Linear oscillator
- Systems of indistinguishable particles

15.1 Introduction

Up to now, we have mainly considered and read about classical statistical mechanics. But sometimes we needed to take quantum mechanics into account in order to have well-behaved partition functions, where 'well-behaved' means in this context that entropy and (free) energies scale linearly with *N*, and also that integrals over phase space are dimensionless.

However that the density functions we have considered so far were essentially *classical*: we have derived Liouville's theorem from the classical (Hamilton) equations of motion, and inferred from that theorem that in equilibrium the density function depends on the Hamiltonian only:

$$\rho(q,p) = \rho[H(q,p)].$$

Now we shall consider statistical mechanics more strictly in the context of quantum mechanics. The analog of the density function now becomes the *density operator*. This operator can be useful when we do not know the actual state of the system, but only the set of possible states which the system can be in, together with the probability for the system to be in any of those states.

The density operator is then

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i| < |$$

where p_i is the normalized probability for the system to be in state $\psi_i\rangle$

$$(\sum_i p_i \equiv 1)$$

From the time-dependent Schrodinger equation

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle$$

and its Hermitian conjugate

$$i\hbar \frac{\partial\langle\psi|}{\partial t} = \langle\psi|\hat{H}$$

which hold for *any* state $|\psi\rangle$, we see that

$$\frac{i\hbar\partial\hat{\rho}}{\partial t} = i\hbar\sum_i p_i\left(\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{\partial}{\partial t}\langle\psi|\right) = \hat{H}\,\hat{\rho} - \hat{\rho}\,\hat{H}$$

From now on, we shall leave the hats from operators unless confusion may arise.

We see that we have an equation quite analogous to Liouville's theorem:

$$\boxed{\dot{\rho} = \frac{i}{\hbar}[H,\rho]}$$

This is called the ***quantum Liouville theorem***. Just as in the classical case, we note that in equilibrium $\dot{\rho}$ must vanish. In case we have a stationary Hamiltonian (i.e. no explicit time dependence), we have

$$\rho = \rho(H)$$

We recall here that for any operator *G*, the expectation value is easily evaluated as

$$< G > = \frac{Tr\,\rho G}{Tr\,\rho}$$

Here, Tr is the *trace* operator. For any orthonormal basis $|\varphi_n\rangle$, it is evaluated as

$$Tr\,A = \sum_n \langle\varphi_n|A|\varphi_n\rangle$$

In a finite-dimensional Hilbert space, the basis is finite, and the trace boils down to adding the diagonal elements of the matrix representation of the operator being traced.

Suppose we have an orthonormal basis set φ_n which forms a basis in our Hilbert space, Then we can express ρ with respect to this basis:

$$\rho_{nm} = \langle\varphi_n|\rho|\varphi_m\rangle$$

This is the matrix representation. In a finite-dimensional Hilbert space, we therefore speak of the density *matrix* rather than an operator. In case we have a state $|\psi\rangle$ which can be expressed in this basis as

$$|\psi > = \sum_n a_n(t)|\varphi_n\rangle$$

we have

$$\rho = |\psi\rangle\langle\psi|$$

The density matrix then reads

$$\rho_{nm} = a_n(t)a_m^*(t)$$

In a many-particle system, the physical wavefunctions have coordinates $\vec{r}_1, \ldots, \vec{r}_N$. Also, spin degrees of freedom might be included. The wavefunction in general can therefore be written as $\psi(x_1, \ldots, x_N)$, where x_i is supposed to include all degrees of freedom of a single particle. Now suppose we have a complete set of basis states $\phi_n(x)$ (n might assume an infinite number of values, even continuum) for a single particle. Then a complete set of states for a system consisting of N particles is

$$\psi_{(n_1 \ldots n_N)}(x_1, \ldots x_N) = \phi_{n_1}(x_1), \ldots, \phi_{n_N}(x_N)$$

A general state of the system is a linear combination of these basis states. In general, such a state is entangled.

15.2 Statistics of the Various Ensembles

The density operator of a quantum system is given as

$$\rho = \delta [H - EI]$$

where I is the unit operator.

In practice, we do not rigorously implement a delta-function, but instead, count the states in a narrow interval $(E, E + \Delta E)$. We can, instead of using the delta-function, also use the theta-function which is constant for all energies smaller than E, and zero for energies above E. As mentioned in the previous chapters, it does not matter which representation we choose because, for large particle numbers, the dominant contributions to the entropy come from energies very close to E in the latter representation.

The entropy is given as

$$S = k_B \ln \Gamma$$

where Γ is the number of states with energy in a narrow band $(E, E + \Delta E)$.

In a basis of eigenstates of the Hamiltonian, the density matrix becomes diagonal

$$\rho_{nn} = \begin{cases} \frac{1}{\Gamma} & for\ E_n < E \\ 0 & for\ E_n \geq E \end{cases}$$

In the canonical ensemble, we have a density operator

$$\rho = Ce^{-\beta \hat{H}}$$

If we express this operator with respect to an energy-basis, that is, an orthonormal basis of eigenfunctions of the Hamiltonian with eigenvalues E_n:

$$\rho_{n,m} = Ce^{-\beta E_n}\delta_{n,m}$$

From this, the normalization is easily found as

$$\frac{1}{C} = Tr\, e^{-\beta \hat{H}} = Q_N(T)$$

The grand canonical ensemble is formulated using the *particle number operator* $\hat{n}$ in addition to the Hamiltonian:

$$\rho = Ce^{-\beta \hat{H}+\beta\mu\hat{n}}$$

In most cases, the particle number operator commutes with the Hamiltonian. The grand canonical partition function is then found again as

$$\frac{1}{C} = Z(\mu, v, T) = \sum_N e^{\beta\mu N} \sum_S e^{-\beta E_s} = \sum_N e^{\beta\mu N} Q_N(T)$$

In order to practice the quantum formulation a bit, we calculate properties for some systems we have considered before in the classical context.

15.3 Electron in a Magnetic Field

The first example is that of an electron in a magnetic field. We consider only the interaction of the magnetic moment with the magnetic field, and not the orbital degrees of freedom (i.e. the motion of the electron, perhaps in some potential). The calculation is most conveniently done in the canonical ensemble.

Considering only a single spin, we have

$$H = -\mu_B(\vec{\sigma}.\vec{B})$$

We work in the representation in which σ_z is diagonal. Then we can use the fact that the exponential of a diagonal operator is again a diagonal operator with the exponentials of its eigenvalues on the diagonal

$$\rho = \frac{e^{-\beta B\mu_B\sigma_z}}{Tr\, e^{-\beta B\mu_B\sigma_z}} = \frac{1}{e^{-\beta B\mu_B} + e^{\beta B\mu_B}} \begin{pmatrix} e^{\beta B\mu_B} & 0 \\ 0 & e^{-\beta B\mu_B} \end{pmatrix}$$

Then we obtain for the average expectation value of σ_z:

$$< \sigma_z > = Tr\,(\rho\sigma_z) = \frac{e^{\beta B\mu_B} - e^{-\beta B\mu_B}}{e^{-\beta B\mu_B} + e^{\beta B\mu_B}} = tanh(\beta\mu_B B)$$

A comparison with classical canonical ensemble shows that these results are correct.

15.4 Self Learning Exercise- I

Q.1 Define density operator.

Q.2 State and prove the *quantum Liouville theorem*.

Q.2 Explain electron in a magnetic field.

Q.4 Prove that

$$\frac{1}{C} = \sum_{N} e^{\beta\mu N}\, Q_N(T)$$

15.5 Free Particle in a Box

Let us consider a free particle in a box, governed by the Hamiltonian

$$H = \sum_{i} \frac{p_i^2}{2m}$$

Inside the cubic box of size L in which the particles move, the potential is zero; outside, we assume periodic boundary conditions. The eigenfunctions which are compliant with these boundary conditions are

$$\psi(\vec{r}) = \left(\frac{1}{L}\right)^{\frac{3}{2}} e^{i(k_x x + k_y y + k_z z)}$$

with $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$. The corresponding energies are

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

We must choose a basis of the Hilbert space in order to evaluate the trace.

First we choose as a basis the eigenfunctions which we denote as$|k\rangle$

$$\langle k|e^{-\beta H}|k'\rangle = e^{\frac{\hbar^2 k^2}{2mk_B T}}\, \delta\left(\vec{k} - \vec{k}'\right)$$

so that the partition function becomes

$$\begin{aligned} Q_T &= Tr\left(e^{-\beta H}\right) \\ &= \sum_{k} \langle k|e^{-\frac{H}{k_B T}}|k'\rangle = \sum_{k} e^{\left(-\frac{\beta\hbar^2 k^2}{2m}\right)} \\ &\approx \frac{L^3}{(2\pi)^3} \int d^3k\, e^{-\frac{\beta\hbar^2 k^2}{2m}} = V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}} \end{aligned}$$

The partition function of a free particle in a box

$$\boxed{Q_T = V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}}}$$

That the transition from the sum to the integral requires an extra factor $L^3/(2\pi)^3$ can be seen as follows. On the grid of k-values, the volume occupied by a k-point is $(2\pi)^3/L^3$. The sum runs over the points in a certain volume. This is then equal to that volume (i.e. $\int d^3k$) divided by the volume per point.

It is instructive to derive the same partition function using the $\vec{r}$ -representation:

$$\begin{aligned}\langle r|e^{-\beta H}|r'\rangle \\ &= \frac{1}{L^3}\sum_k e^{i\vec{k}.(\vec{r}\prime-\vec{r})}e^{-\frac{\hbar^2k^2}{2mk_BT}} \\ &\approx \frac{1}{(2\pi)^3}\int d^3k\, e^{i\vec{k}.(\vec{r}\prime-\vec{r})}e^{-\frac{\hbar^2k^2}{2mk_BT}} \\ &\approx \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}}\exp\left(-\frac{m}{2\beta\hbar^2}|\vec{r}'-\vec{r}|^2\right)\end{aligned}$$

The Fourier integral will be discussed in the exercises. Using this, the partition function can be evaluated as

$$Q_1(T) = \int \langle r|e^{-\beta H}|r'\rangle\, d^3r = V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}}$$

which is obviously the same as the one found above.

The quantity $\langle r|\rho|r'\rangle$which occurs in these expressions (remember $\rho = exp(-\beta H)$ represents the probability density of finding the particle at position $\vec{r}$. Because we have periodic boundary conditions, this must not depend on $\vec{r}$, as we have found.

On the other hand, the expression $\langle r|\rho|r'\rangle$ gives the probability that a particle suddenly moves from $\vec{r}$ to $\vec{r}'$ as a result of a thermal fluctuation.

Let us evaluate the expectation value of the energy. This is most easily evaluated in the $\vec{k}$ representation:

$$< H > = \frac{Tr\left(He^{-\beta H}\right)}{Tr\left(e^{-\beta H}\right)}$$

$$= \frac{1}{Q_1}\left(\frac{V}{(2\pi)^3}\right)\int \hbar^2 k^2 \frac{1}{2m} e^{-\frac{\hbar^2 k^2}{2mk_B T}} d^3k = \frac{3}{2}k_B T$$

that is, equipartition is satisfied. We could also use

$$< H > = -\frac{\partial\, lnTr\,(e^{-\beta H})}{\partial \beta}$$

which leads to the same result.

15.6 Linear Oscillator

Let us consider the case of a linear harmonic oscillator whose Hamiltonian is given by

$$\hat{H} = \frac{1}{2}kq^2 + \frac{1}{2m}p^2$$

With eigenvalues

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

and eigenfunctions

$$\phi_{n(q)} = \frac{\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} H_n(\xi)}{(2^n n!)^{\frac{1}{2}}}\, e^{-\frac{\xi^2}{2}}$$

where

$$\zeta = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} q$$

and

$$H_n(\xi) = (-1)^n e^{\xi^2}\left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$

The matrix elements of the operator $\exp(-\beta H)$ in the q-representation are given by

$$\langle q|\exp(-\beta H)|q'\rangle = \sum_{n=0}^{\infty} \exp(-\beta E_n)\ \varphi_n(q)\varphi_n(q')$$

$$= \sum_{n=0}^{\infty} \frac{\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}}{(2^n n!)}\, e^{-\frac{(\xi^2+\xi'^2)}{2}} e^{\left(-n+\frac{1}{2}\right)\beta\hbar\omega}\, H_n(\xi).H_n(\xi')$$

The summation over n is somewhat difficult to evaluate; nevertheless, the final result is

$$\langle q|\exp(-\beta H)|q'\rangle = \sum_{n=0}^{\infty}\left(\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}\right)^{\frac{1}{2}} e^{\left[-\frac{m\omega}{4\hbar}\{(q+q')^2\tanh\left(\frac{\beta\hbar\omega}{2}\right)+(q-q')^2\coth\left(\frac{\beta\hbar\omega}{2}\right)\}\right]}$$

which gives

$$Tr\exp(-\beta H) = \int_{-\infty}^{\infty}\langle q|\exp(-\beta\hat{H})|q\rangle dq$$

$$= \left(\frac{m\omega}{2\pi\hbar\,sinh\,\beta\hbar\omega}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} e^{\left[-\frac{m\omega}{\hbar}q^2\,tanh\left(\frac{\beta\hbar\omega}{2}\right)\right]}dq$$

$$= \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}}$$

Expression is indeed the *partition function* of a linear harmonic oscillator.

Partition function of a linear harmonic oscillator.

$$Q = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}}$$

At the same time, we find that the *probability density* for the oscillator coordinate to be in the vicinity of the value q is given by

$$\langle q|\hat{\rho}|q\rangle = \left(\frac{m\omega\,tanh\,(\beta\hbar\omega/2)}{\pi\hbar}\right)^{\frac{1}{2}} e^{\left[-\frac{m\omega q^2}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right]}$$

we note that this is a Gaussian distribution in q, with mean value zero and root-mean square deviation

$$q_{rms.} = \left(\frac{\hbar}{2m\omega\tanh\frac{\beta\hbar\omega}{2}}\right)^{\frac{1}{2}}$$

In the classical limit $\beta\hbar\omega \ll 1$, the distribution becomes *purely thermal*—free from quantum effects:

$$\langle q|\hat{\rho}|q\rangle = \left(\frac{m\omega^2}{2\pi kT}\right)^{\frac{1}{2}} e^{[-\frac{m\omega q^2}{2kT}]}$$

with dispersion $1/\left(\frac{m\omega^2}{kT}\right)^{\frac{1}{2}}$. At the other extreme $\beta\hbar\omega \gg 1$ the distribution becomes *purely quantum-mechanical*—free from thermal effects:

$$\langle q|\hat{\rho}|q\rangle = \left(\frac{m\omega^2}{\pi\hbar}\right)^{\frac{1}{2}} e^{[-\frac{m\omega q^2}{\hbar}]}$$

with dispersion $1/\left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}}$.

15.7 Systems of Indistinguishable Particles

We shall now formulate the quantum-mechanical description of a system of N identical particles. To fix the ideas, we start by considering the noninteracting case. Then, the Hamiltonian has the form

$$H = \sum_1^N H_n$$

where H_n only acts on the coordinates of particle n. The coordinates of the particles are denoted by

$$q = (q_1, q_2, \dots);$$

where q_n denotes the coordinate (s) of particle n. The eigenstates of the Hamiltonian then have the form

$$\Psi_E(q) = \prod_{n=1}^{N} u_n(q_n)$$

$$H_n u_n = \varepsilon_n u_n$$

The total energy is given as

$$E = \sum_{n=1}^{N} \varepsilon_n$$

Note that n denotes a particle, not a particular energy level. Now suppose that the particles are identical in that case, the form of the Hamiltonians, and their spectra should be identical. Now suppose that we have N particles with energy E. As each

of the particles occupies energies of the same spectrum, there might be more than one particle in the one state with energy ε_i. We must have:

$$N = \sum_i n_i$$

$$E = \sum_i \varepsilon_i$$

The states can then be written as

$$\Psi_E(q) = \prod_{m=1}^{n_1} u_1(q_m) \prod_{m=1}^{n_2} u_2(q_m) \ldots.$$

Now, if the particles are *identical*, we know that a permutation of them leaves the total Hamiltonian invariant. If this is the case, ***the Hamiltonian commutes with the permutation operator:***

$PH = HP$

If an operator commutes with the Hamiltonian, it must be possible to construct the eigenstates of the Hamiltonian in such a way, that they are simultaneously eigenstates of that operator. You might recall from your mathematics course that any permutation can be written as a product of particle exchanges (a particle exchange means that we exchange a particle pair, *i*; *j*, say). Let us call $P_{i,j}$ a particle exchange for the pair *i, j*. We obviously have $P_{i,j}^2 = 1$. ***Then also the eigenvalues λ of $P_{i,j}$ should satisfy $\lambda^2 = 1$.*** As we furthermore know that, since $P_{i,j}$ is Hermitian, l is real, we must have $\lambda = \pm 1$. We see that the particle wavefunctions are either symmetric under particle exchange ($\lambda = 1$) of antisymmetric ($\lambda = -1$). It turns out that for a particular kind of particles, we have either one or the other possibility. ***Particles whose wavefunction is symmetric with respect to exchange, are called bosons; those which have antisymmetric wavefunctions are called fermions.***

The fact that any permutation operator can be written as a product of exchanges, leads to the conclusion that always

$$\boxed{P\psi_E = \pm\psi_E}$$

This notion directly leads to the conclusion that the microstates are invariant with respect to any permutation of the particles. Therefore, the numbers n_i, which tell us how many particles can be found in state *i*, define a microstate uniquely, and

additional correction factors for proper counting should not be included in sums over the states.

Even if the particles interact, we can use the same representation (although the u_i are no longer eigenstates of single-particle Hamiltonians). The reason why interaction does not matter is that the products of single particle states form a basis of the Hilbert space for many particles, whether they interact or not.

Finally we note that, for fermions, we can construct wavefunctions constructed from single particle states u_i as follows:

$$\psi(q) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_i(q_1)u_i(q_2) & \dots & u_i(q_N) \\ . & . & . \\ u_l(q_1)u_l(q_2) & \dots & u_l(q_N) \end{vmatrix}$$

where the vertical bars denote a determinant. This wavefunction is called a *Slater determinant*. The prefactor follows automatically from the normalization condition (the u_i are considered to be normalized). In the case of Bosons, we have a similar expression, but the minus-signs in evaluating the determinant all turn into plus-signs.

Another way of writing the wavefunction is

$$\psi(q_1, .., q_N) = \sum_p \delta^{|p|} P u_i(q_1)u_j(q_2)..u_l(q_N)$$

where $\sum_p$ denotes a sum over *all possible* permutations, $\delta = 1$ for bosons and -1 for fermions and $[P]$ is the sign of the permutation. The sign of the permutation is determined as the number of exchange operations it is composed of. Note that the permutation operator acts on the *arguments* q_n of the wavefunctions only, not on the labels *i,j,...* Note that this state is not normalized in the case of bosons:

$\langle\psi|\psi\rangle = n_1! n_2!$ ...where n_1 etc. are the occupation numbers of the different states. To see that this factor occurs indeed in the normalization, look at a system consisting of ***two bosons***, both in the same state *u*:

$$\psi = \frac{1}{\sqrt{N!}}[u(q_1)u(q_2) + u(q_2)u(q_1)] = \sqrt{2}\, u(q_1)u(q_2)$$

We see that the norm of this state is 2! = 2. For fermions we do not have this problem, as no two particles can be in the same state.

15.8 The Density Matrix and the Partition Function of a System of Free Particles

We know the wavefunctions for a single particle

$$u_{\boldsymbol{k}}(q) = \frac{1}{L^{\frac{3}{2}}} e^{i\vec{k}.\vec{r}}$$

With the above definition of a many-particle basis function, we must therefore evaluate$\langle \boldsymbol{k}_1, \dots, \boldsymbol{k}_N | exp(-\beta H) | \boldsymbol{k}'_1, \dots, \boldsymbol{k}'_N \rangle$

where the states $|\boldsymbol{k}'_1, \dots, \boldsymbol{k}'_N\rangle$ are (anti)symmetrised states.

In order to evaluate this equation we note the following:

- On the left hand side and on the right hand side, we have actually a sum over all permutations.
- For a particular permutation for *different* $\boldsymbol{k}_i$ on the left hand side, the operator exp(−β*H*) in the middle forces the states on the right hand side to correspond in a one-to-one fashion to those on the left hand side.
- The normalizing prefactors $\frac{1}{\sqrt{N!}}$ on the left and right hand side yield a factor $\frac{1}{N!}$.

Combining all these considerations, we see

that$\langle \boldsymbol{k}_1, \dots, \boldsymbol{k}_N | exp(-\beta H) | \boldsymbol{k}'_1, \dots, \boldsymbol{k}'_N \rangle = e^{\left(-\frac{\hbar^2\left(k_1^2+\cdots+k_N^2\right)}{2mk_BT}\right)} \prod_{i=1}^{N} \delta(k_i - k'_i)$

where the normalization factor $n_1!n_2!\dots$ of the Slater determinant has already be divided out in order to work with normalized states. This factor amounts to 1 if all $\mathbf{k}_i$ are different.

When taking the trace, we must sum over a state $\boldsymbol{k}_1,\dots,\boldsymbol{k}_N$. Note that this sum must include a restriction such that for the set of permutations of the quantum numbers $\boldsymbol{k}_1,\dots,\boldsymbol{k}_N$ *only one* member is chosen, otherwise we are overcounting. But we can relax any such restriction provided we divide by the number of possible permutations

$$\frac{N!}{n_1!\,.\,n_2!\,\dots}$$

Therefore we have as the final result

$$Q_N = \frac{1}{N!}\frac{L^{3N}}{(2\pi)^3}\left\{\int exp\left[-\frac{\hbar^2 k^2}{2mk_BT}\right]d^3k\right\}^N = \frac{1}{N!}\left(\frac{V}{\Lambda^3}\right)^{3N}$$

We see that we have obtained the correct expression of the partition function. Note that we have been sloppy in this calculation: if all **k** would be different, the result would be correct. But by integrating over all possible combinations $\mathbf{k}_{1,\ldots,}\mathbf{k}_N$, we have included the cases where two **k**'s are the same. If there is such overlap, the 3*N*-dimensional integral no longer factorizes into *N* three-dimensional integrals. It turns out that the correction turns out to be very small when $V^{\frac{1}{3}} \gg \Lambda$: then for the vast majority of configurations, no two **k**'s overlap.

Obviously, we could have evaluated this partition function using the coordinate (**r**) basis rather than the **k**-basis. We shall work out here the example of a two-particle system. We first evaluate

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | exp(-\beta H) | \boldsymbol{r}_1, \boldsymbol{r}_2 \rangle = \frac{1}{2}\frac{L^6}{(2\pi)^6}\int \{1 \pm cos[(\boldsymbol{k}_1 - \boldsymbol{k}_2).(\boldsymbol{r}_1 - \boldsymbol{r}_2)]\} exp(-\frac{\beta\hbar^2(k_1^2 + k_2^2)}{2m})\, d^3k_1 d^3k_2$$

In this expression, the first term is the one where the particles are both on the left and right hand side of the matrix element in the same state (both either $\mathbf{k}_1$ or $\mathbf{k}_2$), and the second term corresponds to different states on the left and right hand side of the matrix element – the + sign is for bosons, the - for fermions. Evaluating the integrals we obtain

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | exp(-\beta H) | \boldsymbol{r}_1, \boldsymbol{r}_2 \rangle = \frac{1}{2\Lambda^6}\left(1 \pm \exp\left(-\frac{2\pi \boldsymbol{r}_{12}}{\Lambda}\right)^2\right)$$

Taking the trace means that we must integrate over $\mathbf{r}_1$ and $\mathbf{r}_2$

$$Q_2 = \frac{1}{2\Lambda^6}\int (1 + \exp\left(-\frac{2\pi \boldsymbol{r}_{12}}{\Lambda}\right)^2)\, d^3r_1 d^3r_2 = \frac{1}{2}\left(\frac{V}{\Lambda^3}\right)^2\left[1 \pm \frac{1}{2^{\frac{3}{2}}}\left(\frac{\Lambda^3}{V}\right)\right]$$

We see that the result reduces to the correct partition function for the case where $\Lambda \ll V^{\frac{1}{3}} = L$. The probability density for the particles to be at $\mathbf{r}_1$ and $\mathbf{r}_2$ can be

considered for the boson- end fermi case.

We define the *statistical potential* $v_s(r)$ as

$$e^{-\beta\, v_s(r_{12})} = \rho(\boldsymbol{r_1}, \boldsymbol{r_2})$$

We see that the potential has the correct behaviour in the sense that it prevents fermi particles to come close, and favors bose particles to come close.

It is instructive to repeat the calculation for the two-particle partition function in terms of the **k** basis. ***For bosons, we have a possible state for each combination*** $\mathbf{k}_1, \mathbf{k}_2$. In this case, for $\boldsymbol{k_1} \neq \boldsymbol{k_2}$ the wavefunction is

$$\Psi = \frac{1}{\sqrt{2}}\left[\psi_{k_1}(1)\psi_{k_2}(2) + \psi_{k_1}(2)\psi_{k_2}(1)\right]$$

For $\boldsymbol{k_1} = \boldsymbol{k_2}$, the wavefunction is:

$$\psi = \psi_{\boldsymbol{k_1}}(1)\psi_{\boldsymbol{k_1}}(2)$$

Note that the two expressions differ by a factor $\sqrt{2}$.

For fermions, we have a possible state only when $\boldsymbol{k_1} \neq \boldsymbol{k_2}$

$$\Psi = \frac{1}{\sqrt{2}}\left[\psi_{k_1}(1)\psi_{k_2}(2) - \psi_{k_1}(2)\psi_{k_2}(1)\right]$$

If we calculate the partition function, we must integrate over $\mathbf{k}_1$ and $\mathbf{k}_2$, but we see that we must single out the contributions for $\mathbf{k}_1 = \mathbf{k}_2$. In general, for an operator A which is *diagonal* in phase space we have

$$Tr\, A = \frac{1}{2}\left(\frac{V}{(2\pi)^3}\right)^2 \int A(\boldsymbol{k_1}, \boldsymbol{k_2}) d^3k_1 d^3k_2 \pm \frac{1}{2}\frac{V}{(2\pi)^3}\int A(\boldsymbol{k}, \boldsymbol{k}) d^3k$$

For the trace, this results in

$$Tr\, e^{-\beta H} = \frac{1}{2}\left(\frac{V}{(2\pi)^3}\right)^2 \left(\frac{2\pi m k_B T}{\hbar^2}\right)^3 \pm \frac{1}{2}\frac{V}{(2\pi)^3}\left(\frac{\pi m k_B T}{\hbar^2}\right)^{3/2} = \frac{1}{2}\left(\frac{V}{(2\pi)^3}\right)^2 \left(\frac{2\pi m k_B T}{\hbar^2}\right)^3 \left[1 \pm \frac{1}{2^{\frac{3}{2}}}\frac{\Lambda^3}{V}\right]$$

15.9 Self Learning Exercise- II

Q.1 Evaluate the expectation value of the energy and prove equipartition theorem.

Q.2 Calculate *partition function* of a linear harmonic oscillator.

Q.3 Define particle exchanges operator.

Q.4 Differentiate between bosons and fermions particles.

Q.5 Define and plot *statistical potential* $v_s(r)$

15.10 Summary

In this unit we discussed the concept of quantum statistical mechanics, Density matrix and density operator, various examples as an electron in a magnetic field, a free particle in a box, linear oscillator and systems of indistinguishable particles

15.11 Glossary

Electron: An elementary particle with a unit electrical charge and a mass 1/1837 that of the proton. Electrons surround the atom's positively charged nucleus and determine the atom's chemical properties.

Indistinguishable particles: If a system shows measurable differences when one of its particles is replaced by another particle, these two particles are called distinguishable.

System: That part of an experimental system in which we are primarily interested.

Partition function: A function determined by the probability distribution (over phase space in the classical treatment; over quantum states in the quantum treatment) describing a thermally equilibrated system; many thermodynamic quantities can be expressed in terms of the partition function and its derivatives.

Harmonic oscillator: A harmonic oscillator is a physical system that, when displaced from equilibrium, experiences a restoring force proportional to the displacement. A harmonic oscillator that is displaced and then let go will oscillate sinusoidally. Examples from classical physics are a mass attached to a spring and a simple pendulum swinging through a small angle.

15.12 Answer to Self Learning Exercises

Answer to Self Learning Exercise- I

Ans.1: The density operator is

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i|$$

where p_i is the normalized probability for the system to be in state$|\psi_i\rangle$

$$(\sum_i p_i \equiv 1)$$

Answer to Self Learning Exercise -II

Ans.1: the expectation value of the energy

$$< H > = \frac{Tr\left(He^{-\beta H}\right)}{Tr\left(e^{-\beta H}\right)} = \frac{1}{Q_1}\left(\frac{V}{(2\pi)^3}\right)\int \hbar^2 k^2 \frac{1}{2m} e^{-\frac{\hbar^2 k^2}{2mk_B T}} d^3k = \frac{3}{2}k_B T$$

that is, equipartition theorem.

Ans.2: $Tr\exp(-\beta H) = \int_{-\infty}^{\infty}\langle q|\exp\left(-\beta\hat{H}\right)|q\rangle dq$

$$= \left(\frac{m\omega}{2\pi\hbar\, sinh\, \beta\hbar\omega}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{\left[-\frac{m\omega}{\hbar}q^2\, tanh\left(\frac{\beta\hbar\omega}{2}\right)\right]} dq$$

$$= \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}$$

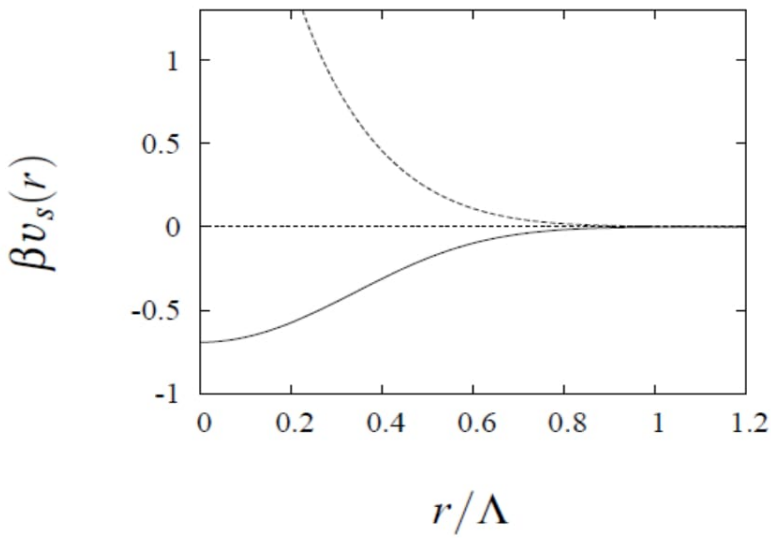
Ans.3: A particle exchange means that we exchange a particle pair, i, *j*. Let us call $P_{i,j}$ a particle exchange for the pair *i, j*. We obviously have $P_{i,j}^2 = 1$. Then also the eigenvalues λ of $P_{i,j}$ should satisfy $\lambda^2 = 1$.

As we furthermore know that, since $P_{i,j}$ is Hermitian, 1 is real, we must have $\lambda = \pm 1$. We see that the particle wavefunctions are either symmetric under particle exchange ($\lambda = 1$) of antisymmetric ($\lambda = -1$). It turns out that for a particular kind of particles, we have either one or the other possibility.

Ans.4 : Particles whose wavefunction is symmetric with respect to exchange, are called *bosons*; those which have antisymmetric wavefunctions are called *fermions*.

Ans.5:

$$e^{-\beta\, v_s(r_{12})} = \rho(\boldsymbol{r_1}, \boldsymbol{r_2})$$



15.13 Exercise

Q.1 Evaluate the density matrix of an electron spin in the representation that makes $\widehat{\sigma_x}$ diagonal.

Q.2 Derive the density matrix ρ for

(i) a free particle

and

(ii) a linear harmonic oscillator in the *momentum* representation

Q.3 Study the density matrix and the partition function of a system of free particles, using the *unsymmetrized* wavefunction instead of the *symmetrized* wavefunction. Show that, following this procedure, one encounters neither the Gibbs' correction factor $\frac{1}{N!}$ nor a spatial correlation among the particles.

Q.4 Show that the quantum-mechanical partition function of a system of N *interacting* particles approaches the classical form.

Q.5 Prove that

$$Tr\, e^{-\beta H} = \frac{1}{2}\left(\frac{V}{(2\pi)^3}\right)^2 \left(\frac{2\pi m k_B T}{\hbar^2}\right)^3 \left[1 \pm \frac{1}{2^{\frac{3}{2}}}\frac{\Lambda^3}{V}\right]$$

References and Suggested Readings

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UNIT -16
The Gibbs Distribution

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16.0 Objectives

Our aim in this chapter is that if a system in equilibrium can be in one of N-states, then we have to find the probability of the system to be found in the state having energy E_n .

It is our objective to find the distribution function for a subsystem. This distribution function is known as “Gibbs distribution”.

16.1 Introduction

In this chapter we wish to consider a general system with a fixed number of particles in thermal equilibrium (The modification to the theory when the number of particles is variable is discussed in unit 17.

- The system may either be isolated from its environment (and therefore at constant energy) or be in contact with a thermal reservoir at temperature T.
- The system at constant energy will in fact never be completely isolated and should therefore be specified as having energy in the range E to $E + \delta E$.
- The energy of the whole system of interest will be written as E.
- The system will not remain in one particular quantum state indefinitely even when in thermal equilibrium but rather will pass through all the quantum states accessible to it as the result of small fluctuations in the surroundings. It is never possible to shield a system from surroundings.
- Since macroscopic properties of a system in thermal equilibrium are independent of time, it should in principle be possible to determine the probability of the system being in a particular quantum state (γ) by making a series of measurements at successive times, provided that the time between measurements was sufficiently long relative to the longest relaxation time of the system. The system contains a constant number of particles at constant volume and is in contact with a thermal reservoir at temperature T.
- The entire system of thermal reservoir and system of interest could be treated as isolated and the properties of the composite system calculated using microcanonical ensemble.
- Alternatively we may consider a set of replicas of the experimental system placed side by side in thermal contact and imagine the whole ensemble to be isolated from its surroundings. Gibbs called this a “Canonical ensemble”.
- There is no restriction on the energy of the experimental system in this case since it may exchange energy with the thermal reservoir.

16.2 The Gibbs distribution

- In this chapter we consider the problem of finding the distribution function for a subsystem, i.e. any macroscopic body which is a small part of some large closed system.
- The most convenient and general method of approaching the solution of this problem is based on the application of the microcanonical distribution to the whole system.
- Distinguishing the body in question from the rest of the closed system, we may consider the system as consisting of these two parts. The rest of system will be called the "Medium" in relation to the body.

The microcanonical distribution can be formulated by writing

$$dW = \text{constant} \times \delta\left(E + E' - E^{(o)}\right) d\Gamma\, d\Gamma' \qquad (1)$$

Where E, $d\Gamma$ and E', $d\Gamma'$ relate to the body and the medium respectively, and $E^{(o)}$ is the given value of the energy of the closed system, which must be equal to the sum $E+E'$ of the energies of the body and the medium. $d\Gamma$ and $d\Gamma'$ represent the numbers of quantum states of the body and the medium respectively.

Our object is to find the probability W_n of a state of the whole system such that the body concerned is in some definite quantum state (with energy E_n) , i.e. a macroscopically defined state.

The microscopic state of the medium is of no interest so that we shall suppose this to be in a macroscopically defined state.

Let $\Delta\Gamma'$ be the statistical weight of the macroscopic state of the medium and let $\Delta E'$ be the range of values of the energy of the medium corresponding to the range $\Delta\Gamma'$ of quantum states.

The required probability W_n can be found by taking $d\Gamma = 1$ in (1), putting $E = E_n$ and integrating with respect to Γ':

$$W_n = \text{constant} \times \int \delta\left(E_n + E' - E^{(0)}\right) d\Gamma'$$

Let $\Gamma'(E')$ be the total number of quantum states of the medium with energy not exceeding E'.

Since the integrand depends only on E', we can change to integration with respect to E', putting $d\Gamma' = \left(\frac{d\Gamma'(E')}{dE'} \right) dE'$.

The derivative $\frac{d\Gamma'}{dE'}$ is replaced by $\frac{e^{S'(E')}}{\Delta E'}$, where $S'(E')$ is the entropy of the medium as a function of its energy; $\Delta E'$ is also a function of E'. Thus we have

$$W_n = \text{constant} \times \int \frac{e^{S'}}{\Delta E'} \delta\left(E' + E_n - E^{(0)}\right) dE'$$

Owing to the presence of the delta function, the result of the integration is simply to replace E' by $E^{(0)} - E_n$:

$$W_n = \text{constant} \times \left(\frac{e^{S'}}{\Delta E'} \right)_{E' = E^{(0)} - E_n} \tag{2}$$

We now use the fact that, since the body is small, its energy E_n is small in comparison with $E^{(0)}$.

The quantity $\Delta E'$ undergoes only a very small relative change when E' varies slightly, and so in $\Delta E'$ we can simply put $E' = E^{(0)}$; it then becomes a constant independent of E_n.

In the exponential factor $e^{S'}$, we must expand $S'\left(E^{(0)} - E_n\right)$ in powers of E_n as far as the linear term:

$$S'\left(E^{(0)} - E_n\right) = S'\left(E^{(0)}\right) - E_n \frac{dS'\left(E^{(0)}\right)}{dE^{(0)}}$$

The derivative of the entropy S' with respect to energy is just $\frac{1}{T}$, where T is the temperature of the system; the temperatures of the body and the medium are the same, since the system is assumed to be in equilibrium.

Thus we have

$$S'\left(E^{(0)} - E_n\right)^0 = S'\left(E^0\right) - \frac{E_n}{k_B T} \tag{3}$$

From (2), we now obtain, (by substituting (3))

$$W_n = A e^{\frac{-E_n}{k_B T}} \tag{4}$$

Where A is a normalization constant independent of E_n. This is one of the most important formulas in statistical physics. ***This distribution is called the Gibbs distribution or canonical distribution.*** It gives the statistical distribution of any macroscopic body which is a comparatively small part of a large closed system.

In classical statistics an expression exactly corresponding to (4) is obtained for the distribution function in phase space:

$$\rho(p,q) = A e^{-E(p,q)/k_B T} \tag{5}$$

Where $E(p,q)$ is the energy of the body as a function of its coordinates and momenta. The normalization constant A in (5) is given by the condition

$$\int \rho dpdq = A \int e^{-E(p,q)/k_B T} dpdq = 1 \tag{6}$$

The normalization constant A is given by the condition

$$\sum_n W_n = 1, \text{ therefore}$$

$$\frac{1}{A} = \sum_n e^{-\frac{E_n}{k_B T}} \tag{7}$$

16.3 The Maxwellian distribution

The energy $E(p,q)$ in the Gibbs distribution formula of classical statistics can always be written as the sum of two parts: the kinetic energy and the potential energy.

If the kinetic and potential energies are denoted by $K(p)$ and $U(q)$ respectively, then $E(p,q) = K(p) + U(q)$

where $K(p) = \frac{p^2}{2m}$, and $U(q)$ is a function of the coordinates of the atoms.

The probability $dW = \rho(p,q)dpdq$

$$= A e^{-U(q)/k_B T} e^{-K(p)/k_B T} dpdq \tag{1}$$

$\rho(p,q)$ is the distribution function in phase space.

That is dW is the product of two factors, one of which depends only on the

coordinates and the other only on the momenta.

This means that the probabilities for momenta and coordinates are independent, in the sense that any particular values of the momenta do not influence the probabilities of the various values of the coordinates, and vice-versa.

Thus the probability of the various values of the momenta can be written

$$dW_p = a\, e^{-K(p)/k_B T} dp \tag{2}$$

and the probability distribution for the coordinates is

$$dW_q = b\, e^{-U(q)/k_B T} dq \tag{3}$$

Since the sum of the probabilities of all possible values of the momenta must be unity (and the same applies to the coordinates), each of the probabilities dW_q must be normalized, i.e. their integrals over all possible values of the momenta and coordinates respectively for the body concerned must be equal to unity.

From these conditions we can determine the constants *a* and *b* in (2) and (3).

Let us consider the probability distribution for the momenta, and once again emphasize the very important fact that in classical statistics this distribution does not depend on the nature of the interaction of particles within the system or on the nature of the external field, and so can be expressed in a form applicable to all bodies. In quantum statistics this statement is not true in general.

We can therefore write the probability distribution for the momenta of each atom separately.

For an atom of mass *m* on the kinetic energy is $\frac{p_x^2 + p_y^2 + p_z^2}{2m}$, where p_x, p_y, p_z are the cartesian components of its momentum, and the probability distribution is

$$dW_p = a\, e^{-\left(p_x^2+p_y^2+p_z^2\right)/2mk_B T} dp_x dp_y dp_z$$

The constant *a* is given by the normalization condition. The integrations over p_x, p_y, p_z are separate; by means of formula

$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$, we find $a = \left(2\pi m k_B T\right)^{-3/2}$, and the momentum probability distribution takes the final form

$$dW_p = \frac{1}{\left(2\pi m k_B T\right)^{3/2}} \; e^{-\left(p_x^2+p_y^2+p_z^2\right)/2mk_BT} \; dp_x dp_y dp_z \tag{4}$$

Changing from momenta to velocities $\left(\vec{p}=m\vec{v}\right)$ we can write the corresponding velocity distribution as

$$dW_{\vec{v}} = \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{\frac{m\left(v_x^2+v_y^2+v_z^2\right)}{2k_BT}} dv_x dv_y dv_z \tag{5}$$

This is the Maxwellian distribution. It again consists of a product of three independent factors

$$dW_{v_x} = \sqrt{\frac{m}{2\pi k_B T}} e^{-mv_x^2/2k_BT} dv_x \; ,....$$

16.4 Self Learning Exercise-I

Q.1 Prove the thermodynamic relation

$$E = -T^2\left(\frac{\partial}{\partial T}\frac{F}{T}\right)_V$$

Where F is free energy, E is the internal energy.

Q.2 Find the mean value of v^2 and v^3 using Maxwellian distribution formula.

16.5 The Gibbs distribution for a variable number of particles

So far we have always tacitly assumed that the number of particles in a body is some given constant, and have deliberately passed over the fact that in reality particles may be exchanged between different subsystems.

In other words, the number N of particles in a subsystem will necessarily fluctuate about its mean value.

In order to formulate precisely what we mean by the number of particles, we shall use the term ‘subsystem’ to refer to a part of the system which is enclosed in a fixed volume. Then N will denote the number of particles within that volume.

The distribution function now depends not only on the energy of the quantum state but also on the number N of particles in the body, and the energy levels E_{nN} are of

course different for different N (as indicated by the suffix N).

The probability that the body contains N particles and is in the n^{th} state will be denoted by W_{nN}.

In this case, the entropy of the medium is now a function not only of its energy E' but also of the number N' of particles in it : $S'=S'\left(E',N'\right)$.

Writing $E'=E^{(0)}-E_{nN}$ and $N'=N^{(0)}-N$ (where N is the number of particles in the body, and $N^{(0)}$ the given total number of particles in the entire closed system, which is large compared with N), we have

$$W_{nN} = \text{Constant} \times \exp\left\{S'\left(E^{(0)}-E_{nN},N^{(0)}-N\right)\right\}; \tag{1}$$

The quantity $\Delta E'$ is regarded as constant.

Next, we expend S' in powers of E_{nN} and N, again taking only the linear terms.

We shall now formally consider N as a further independent variable. Then the total differential of the energy will be written.

$$dE=TdS-PdV+\mu dN \tag{2}$$

Where μ denotes the partial derivative

$$\mu=\left(\frac{\partial E}{\partial N}\right)_{S,V} \tag{3}$$

The quantity μ is called the chemical potential of the body.

From (2), we find

$$dS=\frac{dE}{T}+\frac{P}{T}dV-\frac{\mu}{T}dN$$

$$\left(\frac{\partial S}{\partial E}\right)_{V,N}=\frac{1}{T},\left(\frac{\partial S}{\partial E}\right)_{E,V}=-\frac{\mu}{T}$$

Hence

$$S'\left(E^{(0)}-E_{nN},N^{(0)}-N\right)\simeq S'\left(E^{(0)},N^{(0)}\right)-E_{nN}\frac{\partial S'}{\partial E^{(0)}}-N\frac{\partial S'}{\partial N_0}$$

Or $$S'\left(E^{(0)}-E_{nN},N^{(0)}-N\right)\cong S'\left(E^{(0)},N^{(0)}\right)-\frac{E_{nN}}{T}+\frac{\mu N}{T},$$

the chemical potential μ (and the temperature) being the same for the body and the medium, from the condition of equilibrium.

Thus we obtain for the distribution function the expression

$$W_{nN} = A e^{(\mu N - E_{nN})/k_B T} \tag{4}$$

The normalization constant A can be expressed in terms of the thermodynamic quantities.

By definition the entropy of the body is

$$S = -\langle \log W_{nN} \rangle = -\log A - \frac{\mu \bar{N}}{T} + \frac{\bar{E}}{T}$$

and so

$$T \log A = \bar{E} - TS - \mu \bar{N}$$

But $\bar{E} - TS = F$, and the difference $F - \mu \bar{N}$ is the thermodynamic potential Ω.

Thus $T \log A = \Omega$, and (4) may be rewritten as

$$W_{nN} = e^{(\Omega + \mu N - E_{nN})/k_B T} \tag{5}$$

This is the final formula for the Gibbs distribution for a variable number of particles.

This distribution is sometimes called the 'grand canonical ensemble'.

The normalization condition for the distribution (5) requires that the result of summing the W_{nN} first over all quantum states (for a given N) and then over all values of N should be equal to unity:

$$\sum_N \sum_n W_{nN} = e^{\Omega/k_B T} \sum_N \left(e^{\frac{\mu N}{k_B T}} \sum_N e^{-\frac{E_{nN}}{k_B T}} \right) = 1$$

Hence we obtain the following expression for the thermodynamic potential Ω:

$$\Omega = -T \log \sum_N \left[e^{\frac{\mu N}{k_B T}} \sum_n e^{-\frac{E_{nN}}{k_B T}} \right] \tag{6}$$

This formula together with $F = -T \log \sum_n e^{-E_n/k_B T}$ can be used to calculate the thermodynamic quantities for specific bodies.

In classical statistics the probability distribution has the form

$$dW_N = \rho_N \, dp^{(N)} dq^{(N)}$$

Where $\rho_N = (2\pi\hbar)^{-s} e^{\frac{[\Omega+\mu N - E_N(p,q)]}{k_B T}}$ (7)

The variable N is written as a subscript to the distribution function, and the same letter is written as a superscript to the element of phase volume in order to emphasize that a different phase space (of 2*s* dimensions) corresponds to each value of N. The formula for Ω correspondingly becomes :

$$\Omega = -k_B T \log\left\{\sum_N e^{\frac{\mu N}{k_B T}} \int' e^{-\frac{E(p,q)}{k_B T}} d\Gamma_N\right\}$$

The prime($'$)to the integral indicates that we must integrate over those regions of the phase space corresponding the different states of the body.

16.6 Derivation of the thermodynamic relations from the Gibbs distribution

The key principle of statistical mechanics is as follows :

If a system in equilibrium can be in one of the N-states, then the probability of the system having energy E_n is $Ae^{\frac{-E_n}{k_B T}}$ where

$$A = \frac{1}{\sum_n e^{-\frac{E_n}{k_B T}}} \quad (1)$$

or $$W_n = \frac{1}{Q} e^{-\frac{E_n}{k_B T}} \quad (2)$$

$$\left(A = \frac{1}{Q}\right)$$

Where $Q = \sum_{n=1}^{N} e^{-\frac{E_n}{k_B T}}$. Temperature is measured in Kelvin unit, k is Boltzmann's constant. Q is called the "Partition function".

From the basic principle of statistical mechanics, once

$Q = \sum_n e^{-\frac{E_n}{k_B T}}$ is known, all thermodynamic properties can be found.

We define F, the Helmholtz free energy so that

$$Q = \sum_n e^{-\frac{E_n}{k_B T}} \equiv e^{-\frac{F}{k_B T}} \tag{4}$$

$$F = -k_B T \ln Q = -k_B T \ln\left(\sum_n e^{-\frac{E_n}{k_B T}} \right) \tag{5}$$

$S =$ entropy is defined as $-k_B \sum_n W_n \ln \mathrm{W}_n$ (6)

Where $W_n = \frac{1}{Q} e^{-\frac{E_n}{k_B T}}$

From (5) it can be seen that

$$-\left(\frac{\partial F}{\partial T}\right)_V = -k_B \sum_n \left[\frac{1}{Q} e^{-\frac{E_n}{k_B T}} \left\{ -\frac{E_n}{k_B T} - \ln Q \right\} \right] = S \tag{7}$$

P=Pressure = $\sum_n -W_n \frac{\partial E_n}{\partial V} = -\left(\frac{\partial F}{\partial V}\right)_T$

U=average energy $= \frac{1}{Q} \sum_n E_n . e^{-\frac{E_n}{k_B T}}$

But $\frac{\partial Q}{\partial T} = \frac{1}{k_B T^2} E_n e^{-\frac{E_n}{k_B T}}$

Therefore $U = \frac{kT^2}{Q} \frac{\partial Q}{\partial T} = -T^2 \frac{\partial}{\partial T}\left(\frac{F}{T}\right) = \frac{\partial}{\partial\left(\frac{1}{T}\right)}\left(\frac{F}{T}\right)$

Since $S = -\frac{\partial F}{\partial T}$, $U = F + TS$

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V = \frac{\partial F}{\partial T} - \frac{\partial}{\partial T}\left(T \frac{\partial F}{\partial T}\right)$$

$$= \frac{\partial F}{\partial T} - \frac{\partial F}{\partial T} - T \frac{\partial^2 F}{\partial T^2}$$

$$= -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V$$

16.7 Illustrative Examples

Example16.1 Consider a system of harmonic oscillators in thermal equilibrium. Find the partition function Q, free energy F, average energy of the system of oscillators.

Sol. Assuming that the oscillators do not interact with each other, but only with the surrounding medium (heal bath)

Since each oscillator is independent, one can find F_i of the i^{th} oscillator and then

$$F = \sum_{i=1}^{M} F_i \qquad \text{(M Oscillators)}$$

$$Q_i = \sum_n e - \frac{E_n^i}{k_B T}$$

$$E_n^i = hw_i\left(n + \frac{1}{2}\right) \qquad \text{(n = 0, 1, 2, ...)}$$

$$Q_i = \sum_n e^{\frac{-hw_i\left(n+\frac{1}{2}\right)}{k_B T}}$$

$$= \frac{e^{-hw_i/2k_B T}}{1 - e^{-hw_i/2k_B T}}\left[\frac{1}{(1 - e^{-hw_i/2k_B T})} = 1 + e^{-\frac{hw_i}{k_B T}} + ...\right]$$

$$F_i = -k_B T \ln Q_i = \frac{hw_i}{2} + k_B T \ln\left(1 - e^{-hw_i/2k_B T}\right)$$

$$U_i = \frac{1}{Q_i}\sum_n E_n^i e^{-E_n^i/k_B T} = \frac{\partial}{\partial\left(\frac{1}{T}\right)}\frac{F_i}{T}$$

$$= \frac{hw_i}{2} + \frac{hw_i e^{-hw_i/k_B T}}{1 - e^{-hw_i/2k_B T}} = hw_i + \frac{hw_i}{e^{hw_i/2k_B T} - 1}$$

$$F = \sum_i F_i = \sum_i \left[\frac{hw_i}{2} + k_B T \ln\left(1 - e^{-hw_i / k_B T}\right) \right]$$

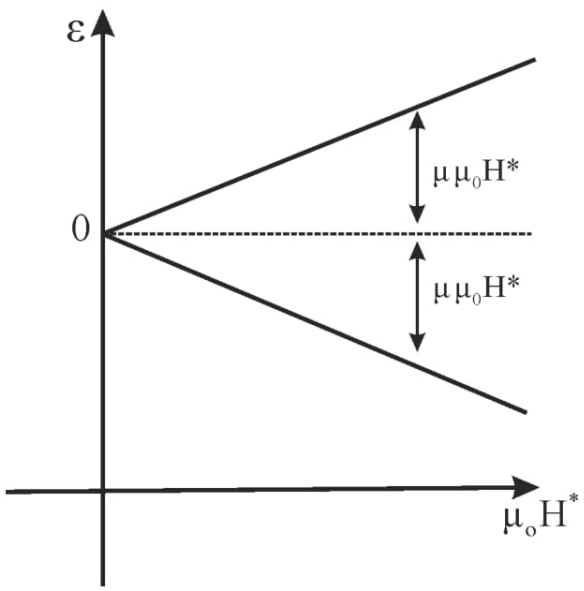
$$U = \sum_i U_i = \sum_i \left[\frac{hw_i}{2} + \frac{hw_i}{e^{hw_i / 2k_B T} - 1} \right]$$

Note that the contribution to F of the i^{th} oscillator is negligible if $hw_i >> k_B T$ (except for the $\frac{hw_i}{2}$ term)

At low temperature the high frequency modes are "frozen out" and do not contribute to the specific heat.

Example16.2 Consider a two level system of a nucleus of spin $\frac{1}{2}$ in a magnetic field. Find the mean energy of the system.

Sol. The energy level is two-fold degenerate in zero field but separates into two non-degenerate levels in a magnetic field $(\mu_0 \mathrm{H}^*)$ with energies $\pm\mu\mu_0 \mathrm{H}^*$ where μ is the magnetic moment of the nucleus (see figure).



The energy zero is taken at zero field value and the splitting of the levels (Δ) is given by

$$\Delta = 2\mu\mu_0 \mathrm{H}^*$$

The single-particle partition function is now

$$Z = e^{-\beta\Delta/2} + e^{\beta\Delta/2}, \qquad \left(\beta = \frac{1}{k_B T}\right)$$

The mean energy of the system is

$$\overline{E} = \frac{N\Delta\left(1 - e^{\beta\Delta}\right)}{2\left(1 + e^{\beta\Delta}\right)}$$

Example 16.3 Find the partition function for N weakly coupled harmonic oscillators.

Sol. The energy levels of the individual oscillators are given by quantum mechanics to be

$$\varepsilon = \left(n + \frac{1}{2}\right)\varepsilon_0 \qquad ;\varepsilon_0 = h\upsilon \qquad \text{n=0 ,1,2,…..}$$

Then the partition function for a single particle is

$$\mathcal{z} = \sum_n e^{-\left(n+\frac{1}{2}\right)\beta\varepsilon_0} = e^{-\frac{\beta\varepsilon_0}{2}}\left(1 + e^{-\beta\varepsilon_0} + e^{-2\beta\varepsilon_0} + \ldots\right)$$

$$\text{or } \mathcal{z} = \frac{e^{-\frac{\beta\varepsilon_0}{2}}}{1 - e^{-\beta\varepsilon_0}}$$

$$\ln Z = N \ln \mathcal{z} = -N\left[\frac{\beta\varepsilon_0}{2} + \ln\left(1 - e^{-\beta\varepsilon_0}\right)\right]$$

The mean energy is

$$\overline{E} = -\left(\frac{\partial}{\partial\beta}\ln Z\right)_v = N\varepsilon_0\left(\frac{1}{2} + \frac{1}{e^{\beta\varepsilon_0} - 1}\right)$$

which is equivalent to

$$\overline{E} = \frac{N\varepsilon_0}{2}\coth\left(\frac{\beta\varepsilon_0}{2}\right)$$

Example16.4 Show that in the high-temperature limit the heat capacity of a two level system is proportional to the inverse square of the temperature.

Sol. The mean energy of the system is defined as

$$\bar{E} = \frac{\sum_r E_n e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}$$, where E_r is the energy of the system in state *r*.

Therefore

$$C_V = \left(\frac{\partial \bar{E}}{\partial T}\right)_V$$

$$= \left(\frac{\partial \bar{E}}{\partial \beta}\right)_V \left(\frac{\partial \beta}{\partial T}\right)$$

$$= k_B \beta^2 \left(\frac{\partial^2}{\partial \beta^2} \ln Z\right)_V$$

$$= N k_B \left(\frac{\varepsilon}{k_B T}\right)^2 \cdot \frac{e^{\beta\varepsilon}}{\left(1 - e^{\beta\varepsilon}\right)^2}$$

In the high temperature limit

$$C_V = \left(\frac{N\varepsilon^2}{4k_B}\right) T^{-2} \qquad (\beta \to 0)$$

In the helium region (4K) the thermal capacity may increase due to this term.

Example.16.5 Find an expression for the entropy of a system of one-dimensional simple harmonic oscillators as function of temperature.

Sol. The partition function for a single particle is

$$\mathcal{Z} = \frac{e^{-\beta \varepsilon_0 / 2}}{1 - e^{-\beta \varepsilon_0}}$$

and $\ln Z = N \ln \mathcal{Z} = -N\left[\frac{\beta \varepsilon_0}{2} + \ln\left(1 - e^{-\beta \varepsilon_0}\right)\right]$

Therefore $F = -k_B T \ln Z,$

and $S = -\left(\frac{\partial F}{\partial T}\right)_V = -\left(\frac{\partial F}{\partial \beta}\right)_V \left(\frac{d\beta}{dT}\right)$

Therefore

$$\frac{S}{Nk} = \frac{\beta\varepsilon_0}{\left[\exp(\beta\varepsilon_0) - 1\right]} - \ln\left[1 - \exp(-\beta\varepsilon_0)\right]$$

16.8 Self Learning Exercise-II

Q.1 If thermodynamic potential ϕ is defined as

$$\phi = E - TS + PV$$

$$= F + PV$$

$$= W - TS$$

Then prove that

$$W = -T^2 \frac{\partial}{\partial T}\left(\frac{\phi}{T}\right)_P$$

Q.2 Calculate the values of Δ/kT for a nucleus of spin $\frac{1}{2}$ with magnetic moment $5\times10^{-24} JT^{-1}$ in a field of 1T(10 kG) at a temperature of 1K and repeat the calculation for an ion with magnetic moment $9\times10^{-24} JT^{-1}$.

Q.3 The temperature of the chromospheres of the sun is approximately 5000 K. Find the relative number of hydrogen atoms in the energy levels with n = 1, 2, 3, 4. The Rydberg constant is $1.1\times10^7\, m^{-1}$.

16.9 Summary

In this chapter we have found the distribution function for a subsystem, i.e. any macroscopic body which is a small part of some large closed system: (body in question plus rest of the system called the "medium").

The most convenient and general method of approaching the solution of this problem is based on the application of the micro canonical distribution to the whole system.

Our object has been to find the probability W_n of a state of the whole system such that the body concerned is in some definite quantum state (with energy E_n). The microscopic state of the medium is of no interest, so that we shall suppose this to be in a macroscopically defined state. According to Gibbs distribution formula-

If a system in equilibrium can be in one of N states, then the probability of the system having energy E_n is

$$W_n = \frac{1}{Q} e^{-\frac{E_n}{k_B T}}$$

Where T is the temperature in energy unit, $Q = \sum_{n=1}^{N} e^{-\frac{E_n}{k_B T}}$ is called the "partition function".

If we take $|i\rangle$ as a state with energy E_i and A as a quantum-mechanical operator for a physical observable, then the expected value of the observable is

$$< A >= \frac{1}{Q} \sum_{|i\rangle} \langle i | A | i \rangle e^{-\frac{E_i}{k_B T}}$$

This fundamental law is the key principle of statistical mechanics and is the summit of statistical mechanics.

16.10 Glossary

Fluctuation :An irregular rising and falling in number or amount; a variation

Chromospheres :A reddish gaseous layer immediately above the photosphere of the sun or another star which, together with the corona ,constiyutes its outer atmosphere the corona, constitutes its outer atmosphere.

Precisely: Exactly (used to emphasize the complete accuracy or truth of statement)

Macroscopic :Relating to large-scale or general analysis.

16.11 Answers to Self Learning Exercises

Answer to Self Learning Exercise-II

Ans.2: See the solution of ExampleNo.16.2

$\frac{\Delta}{kT} = \frac{2u_0 H^*}{kT} = 7 \times 10^{-4}$ for the nucleus.

Therefore it is still in the high temperature limit.

$\frac{\Delta}{kT} = 1.4$ for the ion, so the full expression for the thermal capacity is

required.

Ans.3: $\varepsilon_n = -\frac{hR_\infty}{n^2}$ is the energy of the n^{th} energy level and it is $2n^2$ degenerate. Therefore

$$\frac{P_n}{P_1} = \frac{g_n \exp(-\beta\varepsilon_n)}{g_1 \exp(-\beta\varepsilon_1)} = n^2 \exp\left[\beta\left(\varepsilon_1 - \varepsilon_n\right)\right]$$

$$P_4 : P_3 : P_2 : P_1 = 2\times10^{-10} : 4\times10^{-12} : 2\times10^{-10} : 1$$

(The upper levels are spongely populated even at 5000 K)

16.12 Exercise

Q.1 Prove the following thermodynamic formulae.

$$\mu = \left(\frac{\partial W}{\partial N}\right)_{S,P} = \left(\frac{\partial F}{\partial N}\right)_{T,V} = \left(\frac{\partial \phi}{\partial N}\right)_{P,T}$$

Q.2 The moment of inertia of a molecule is $4.6\times10^{-48}\ \mathrm{k}\,g\,\mathrm{m}^2$. Find the relative populations of the J=0,1,2,3,4 rotational energy levels at 300 K. At what temperature are the J = 2 and J = 3 levels equally populated ?

Q.3 Find the specific heat of an ideal gas in the extreme relativistic case, where the energy of a particle is related to its momentum by $\varepsilon = cp$, c being the velocity of light.

Q.4 Deduce Gibbs distribution formula.

Q.5 Find the number of impacts of gas molecules on unit area of the wall per unit time for which absolute magnitude of velocity lies between v and v +dv

16.13 Answers to Exercise

Ans.1: Hint : $dW = TdS + VdP + \mu dN$

$$dF = -SdT - PdV + \mu dN$$

$$d\phi = -SdT + VdP + \mu dN$$

μ is chemical potential.

Ans.2: $\frac{P_J}{P_0} = (2\mathrm{J}+1)\exp\left[\frac{-J(J+1)h^2}{8\pi^2 kTI}\right]$, I is moment of inertia.

Therefore $P_4 : P_3 : P_2 : P_1 : P_0 = 3\times10^{-2} : 0.2 : 0.9 : 1.6 : 1$

Notice that more molecules are in the first rotational energy level than in the ground state.

For equal populations

$$7\exp\left(-\frac{12h^2}{8\pi^2 IkT}\right) = 5\exp\left(-\frac{6h^2}{8\pi^2 IkT}\right)$$

Therefore $T = 1.5\times10^3 K$

Ans.3: Hint $F = -NkT\log\frac{eV}{N(2\pi\hbar)^3}\int_0^\infty e^{-\frac{cp}{kT}}.4\pi p^2 dp$

or, after carrying out the integration

$$F = -NkTog\left(\frac{AVT^3}{N}\right)$$

Where A is a constant. The specific heat is therefore $C_V = 3$, Which is twice the value for a non-relativistic monatomic gas.

Ans.5: $d\upsilon = \frac{N}{V}\pi\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2T}} v^3 dv$

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UNIT- 17
Ideal Gases: The Boltzmann distribution

Structure of the Unit

17.0 Objectives

17.1 Introduction

17.2 The Boltzmann distribution

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References and Suggested Readings

17.0 Objectives

Our objective are to deduce Boltzmann's distribution of molecules of an ideal gas among various states by making use of Gibbs distribution function. We shall use Boltzmann's distribution formula for the momentum and velocity distribution functions

17.1 Introduction

The kinetic theory of the classical perfect gas (largely due to Maxwell and Boltzmann) was the first statistical theory to be introduced into physics. The equilibrium results of kinetic theory can now all be obtained as special cases of the general results of statistical mechanics but the detailed nature of the kinetic theory

can give added insight into processes such as the pressure exerted by a gas on the wall of a container. The statistical nature of the kinetic theory should be clear from the discussion given in this chapter. An individual molecule will change its velocity after each collision. Only the probability of the molecule being found to have a given velocity (or small range of velocities) can be specified, but for a gas in thermal equilibrium the fraction of the molecules within the given range of velocities remain constant. The equilibrium results of kinetic theory will be discussed in this chapter. We will discuss Boltzmann distribution for ideal gases in equilibrium as well as in non-equilibrium.

17.2 The Boltzmann Distribution

One of the most important subjects of study in statistical physics is an "ideal gas". ***By ideal gas we mean a gas in which the interaction between the particles (molecules) is so weak as to be neglected.***

Physically, this approximation may be allowable either because the interaction of particles is small whatever the distances between them or because the gas is sufficiently rarefied. In this case the rarefaction of the gas results in its molecules being almost always at considerable distances apart, such that the interaction forces are quite small.

The absence of interaction between the molecules enables the quantum mechanics problem of determining the energy levels E_n of the gas as a whole to be reduced to that of determining the energy levels of a single molecule. These levels will be denoted by E_k, the suffix k representing the set of quantum numbers which define the state of the molecule. The energies E_n are then given by the sums of the energies of various molecules.

It must be remembered, however that, even when there is no direct force interaction, quantum mechanics gives a peculiar mutual effect of particles that are in the same quantum state (called the 'exchange effect'). For example, if particles obey Fermi statistics, this effect has the result that no more than one particle can be in each quantum state at one time; a similar effect but in a different form occurs for particles which obey Bose statistics.

Let η_k be the number of particles in a gas which are in the k^{th} quantum state; the numbers η_k are called the 'occupation numbers' of the various quantum states.

We consider the case in which the mean values $\overline{\eta}_k$ of these numbers satisfy the condition for all k

$$\overline{\eta}_k << 1 \tag{1}$$

Physically this case corresponds to a sufficiently rarefied gas. In practice this condition is satisfied for all ordinary molecular or atomic gases. This condition would be violated only at such high densities that the matter concerned could not be regarded as an ideal gas.

The condition $\overline{\eta}_k << 1$ for the mean occupation numbers signifies that in fact not more than one particle is in each quantum state at any instant. Consequently, we may neglect not only the direct forces of interaction of the particles but also their indirect quantum interactions mentioned above.

This in turn enables us to apply the Gibbs distribution formula to the individual molecules. This is because the Gibbs distribution has been derived for bodies which are relatively small, but at the same time macroscopic, parts of large closed system.

The macroscopic nature of these bodies made it possible to regard them as quasi-closed, i.e. to neglect to some extent their interaction with other parts of the system. In the case under consideration the separate molecules of the gas are quasi-closed, although they are certainly not macroscopic bodies.

Applying the Gibbs distribution formula to the gas molecules, we can say that the probability that a molecule is in the k^{th} state is proportional to $e^{-\varepsilon_k / k_B T}$, and therefore so is the number $\overline{n}_k$ of molecules in that state, i.e.

$$\boxed{\overline{n}_k = a\, e^{-\frac{\varepsilon_k}{k_B T}}} \tag{2}$$

Where a is a constant given by the normalization condition

$$\boxed{\sum \overline{n}_k = N} \text{ (N being the total number of particles in the gas).} \tag{3}$$

The distribution of molecules of an ideal gas among the various states that is given by formula (2) is called "Boltzmann distribution"

The constant coefficient in (2) can be expressed in terms of the thermodynamic quantities of the gas.

To do this we shall give another derivation of the formula, based on the application of the Gibbs distribution function to the assembly of all particles in the gas that are in a given quantum state. We are able to do this (even if the numbers $\bar{n}_k$ are not small) since there is no direct force of interaction between these particles and the remainder (or between any of the particles in an ideal gas), and quantum exchange effects occur only for particles in the same state.

Recalling Gibbs distribution formula for a variable number of particles viz.

$$W_{nN} = e^{(\Omega+\mu N-E_n N)/k_B T}$$

We put $E=n_k\varepsilon_k$, $N=n_k$ and adding the suffix k to Ω in the above formula for Gibbs distribution, we find the probability distribution for various values of n_k as

$$W_{n_k} = e^{\{\Omega_k+n_k(\mu-\varepsilon_k)\}/k_B T} \tag{4}$$

In particular, $W_0 = e^{\frac{\Omega_k}{k_B T}}$ is the probability that there are no particles in the state concerned.

In the case of interest here, for which $\bar{n}_k << 1$, the probability W_0 is almost unity, and so in the expression $W_1 = e^{\{\Omega_k+n_k(\mu-\varepsilon_k)\}/k_B T}$ for the probability of finding one particle in the kth state. We can put $W_0 \cong e^{\Omega_{k/k_B T}} = 1$

Then $W_1 = e^{(\mu-\varepsilon_k)/k_B T}$

The probabilities of values $n_k > 1$ must be taken as zero in the same approximation.

Hence $\bar{n}_k = \sum_{n_k} W_{n_k} n_k = W_0.0 + W_1.1$,

$$\bar{n}_k = e^{(\mu-\varepsilon_k)/k_B T} \tag{5}$$

Thus the coefficient in (2) is expressed in terms of chemical potential of the gas, viz. $a = e^{\mu/k_B T}$

The Boltzmann distribution in classical statistics

If the motion of gas molecules (and of the atoms in them) were subject to classical mechanics, we could use, instead of the distribution of molecules in phase space, i.e. over momenta and coordinates.

Let dN be the mean number of molecules "contained" in a volume element of phase space of the molecule, dpdq = $dp_1.....dp_r dq_1....dq_r$ (r being the number of degrees of freedom of the molecule).

We may write this

$$dN = n(p,q)\,d\tau\,, \quad d\tau = \frac{dp\,dq}{(2\pi\hbar)^r} \tag{1}$$

and call $n(p,q)$ the density in phase space.

We then have $n(p,q) = e^{[\mu-\varepsilon(p,q)]/k_B T}$ (2)

Where $\varepsilon(p,q)$ is the energy of the molecule as a function of the coordinates and momenta of its atoms.

Usually, however, it is not the entire motion of the molecule which is quasi-classical, but only the motion corresponding to some of its degrees of freedom. For example, in a gas which is not in an external field, the translational motion of molecules is always quasi-classical.

The kinetic energy of the translational motion then appears in the energy ε_k of the molecule as an independent term, while the remaining part of the energy does not involve x, y, z and $p_x, p_y p_z$.

This enables us to separate from the general formula for the Boltzmann distribution a factor which gives the distribution of the gas molecules with respect to these variables.

The distribution of the molecules in the volume occupied by the gas is clearly just a uniform distribution, and we obtain for the number of molecules per unit volume with momenta (of the translational motion) in given intervals dp_x, dp_y, dp_z, the Maxwillian distribution:

$$dN_{\vec{p}} = \frac{N}{V} a\, \exp\left[-\left(p_x^2 + p_y^2 + p_z^2\right)/2mk_B T\right] dp_x dp_y dp_z$$

To determine the constant *a*, we use the normalization condition:-

$$N = \frac{N}{V} aV \iiint \exp\left(-p_x^2 - p_y^2 - p_z^2\right)/2mk_B T \;\; dp_x dp_y dp_z$$

$$N = \frac{N}{V} aV \left(\sqrt{\pi.2mk_B T}\right)^3$$

$$\therefore \qquad a = \frac{1}{\left(2\pi m k_B T\right)^{3/2}}$$

$$\therefore \qquad dN_{\vec{p}} = \frac{N}{V}\frac{1}{\left(2\pi m k_B T\right)^{3/2}} \exp\left[-\left(p_x^2 + p_y^2 + p_z^2\right)/2mk_B T\right].dp_x dp_y dp_z \qquad (3)$$

$$\boxed{dN_V = \frac{N}{V}\frac{m^{3/2}}{\left(2\pi k_B T\right)^{3/2}} \exp\left[-m\left(v_x^2 + v_y^2 + v_z^2\right)/2mk_B T\right] dv_x dv_y dv_z} \qquad (4)$$

(m being the mass of the molecule), normalized to $\frac{N}{V}$ particles per unit volume.

Next, we consider a gas in an external field, in which the potential energy of a molecule depends only on the coordinates of its centre of mass: $u = u\left(x, y, z\right)$ (for example, a gravitational field).

The Maxwellian distribution for the velocities of the molecules remains unchanged, while the distribution for the coordinates of the centre of mass is given by

$$dN_{\vec{v}} = n_0 e^{-u(x,y,z)/k_B T} dV \qquad (5)$$

This formula gives the number of molecules in an element of volume $dV = dx\,dy\,dz$.

The quantity

$$n\left(\vec{r}\right) = n_0 e^{-u(x,y,z)/k_B T} \qquad (6)$$

is the number density of the particles. The constant n_0 is the density at points where u=0. Formula (6) is known as ***Boltzmann's formula.***

In particular, in a uniform gravitational field along the Z-axis, u=mgZ and the gas density distribution is given by the ***barometric formula:***

$$n\left(z\right) = n_0\, e^{-mg\,z/k_B T} \qquad (7)$$

Where n_0 is the density at the level z = 0.

At large distance from the earth, its gravitational field must be described by the exact Newtonian expression, the potential energy u vanishing at infinity, but a finite quantity cannot be distributed in an infinite volume with a density which is nowhere zero.

This means that in a gravitational field a gas (such as the atmosphere) cannot be in equilibrium and must be continuously dissipated into space.

17.3 Illustrative Example

Example17.1 The mean value of a quantity such as x^n is defined in terms of the distribution function f(x) to be:

$$\overline{x_n} = \frac{\int x^n f(x)dx}{\int f(x)dx}$$

Where the integral extends over the whole range of x. Using the above definition we can find the mean value of the velocity.

Sol.

$$\overline{v_x} = \frac{\int_{-\infty}^{\infty} v_x e^{-\frac{mv_x^2}{2k_BT}} dv_x}{\int_{-\infty}^{\infty} e^{-\frac{mv_x^2}{2k_BT}} dv_x} = 0$$

As may be seen immediately since the numerator is the product of an odd function with an even function. Similarly the other components of the velocity are zero and in general

$$\overline{v^n} = 0 \ \ (n \text{ odd})$$

17.4 Self Learning Exercise-I

Section A : Very Short Answer Type Questions

Q.1 What is the the mean translational energy of a particle.

Section B : Short Answer Type Questions

Q.2 Find the mean square velocity

Q.3 Write the Maxwellian distribution for velocities in spherical coordinates.

17.5 Boltzmann Distribution for Ideal Gases not in equilibrium

The Boltzmann distribution can also be derived in a quite different manner,

directly from the condition of maximum entropy of the gas as a whole, regarded as a closed system.

Any macroscopic state of an ideal gas may be described as follows.

Let us distribute all the quantum states of an individual particle of the gas among groups each containing neighboring states (which, in particular, have neighboring energy values), both the number of states in each group and number of particles in these states being still very large.

Let the groups of states be numbered $j=1,2,....,$ and let G_j be the number of states in group j, and N_j the number of particles in these states.

Then the set of numbers N_j will completely describe the macroscopic state of the gas.

The problem of calculating the entropy of the gas reduces to that of determining the statistical weight ΔT of a given macroscopic state, i.e. the number of microscopic ways in which this state can be realized. Regarding each group of N_j particles as an independent system and denoting its statistical weight by $\Delta\Gamma_j$, we can write

$$\Delta\Gamma = \prod_j \Delta\Gamma_j \tag{1}$$

Thus the problem reduces to that of calculating the $\Delta\Gamma_j$.

In Boltzmann statistics the mean occupation numbers of all quantum states are small in comparison with unity. This means that the numbers of particles N_j must be small compared with the numbers of states $G_j\left(N_j << G_j\right)$, but of course themselves still large.

The smallness of the mean occupation numbers enables us to suppose that all particles are entirely independently distributed among the various states.

Placing each of the N_j particles in one of the G_j states, we obtain altogether $G_j^{N_j}$ possible distributions.

But among these the distributions which differ only by a permutation of particles are identical, since the particles themselves are identical.

The number of permutations of N_j particles is $N_j!$, and so the statistical weight of the distribution of N_j particles among G_j states is

$$\Delta\Gamma_j = \frac{G_j^{N_j}}{N_j!} \tag{2}$$

The entropy of the gas is calculated as the logarithm of the statistical weight:

$$S = \log \Delta\Gamma = \sum_j \log \Delta\Gamma_j$$

Since the numbers N_j are large, we can use the approximate formula whose derivation is given below:

$\log N! = \log 1 + \log 2 + ... + \log N$ may be replaced by the integral

$$\int_0^N \log x\, dx = N \log N - N = \log N^N - N \log e$$

$$= \log\left(\frac{N}{e}\right)^N \tag{3}$$

Using this approximate formula for $\log N_j!$, we find

$$\delta = \sum_j \left\{ \log G_j^{N_j} - \log\left(\frac{N_j}{e}\right)^{N_j} \right\}$$

$$= \sum_j \log\left(\frac{G_j . e}{N_j}\right)^{N_j}$$

$$\delta = \sum_j N_j \log\left(\frac{eG_j}{N_j}\right) \tag{4}$$

This formula determines the entropy S of an ideal gas in any macroscopic state defined by the set of numbers N_j.

It may be rewritten by using the mean numbers $\bar{n}_j$ of particles in each of the quantum states in group j : $\bar{n}_j = \frac{N_j}{G_j}$. Then

$$S = \sum_j G_j \bar{n}_j \log\left(\frac{e}{\bar{n}_j}\right) \tag{5}$$

If the motion of the particles is quasi-classical, then in this formula we can change to the particle distribution in phase space.

Let the phase space of a particle be divided into regions $\Delta p^{(j)}\,\Delta q^{(j)}$, each of which is small but nevertheless contains a large number of particles.

The numbers of quantum states belonging to these regions are

$$G_j = \frac{\Delta p^{(j)} \Delta q^{(j)}}{\left(2\pi\hbar\right)^r} = \Delta\tau^{(j)}, \tag{6}$$

where r is the number of degrees of freedom of the particle.

The numbers of particles in these states may be written as

$N_j = n\left(p,q\right)\Delta\tau^{(j)}$, where

$n\left(p,q\right)$ is the particle density distribution in phase space.

Substituting these expressions in (5), and using the fact that the regions $\Delta\tau^{(j)}$ are small in size and large in number to replace the summation over j by integration over the whole phase space of the particle,

$$S = \int n \log\left(\frac{e}{n}\right) d\tau \tag{7}$$

In a state of equilibrium, the entropy must be a maximum (as applied to the ideal gas, this statement is sometimes called ***Boltzmann's H-theorem***).

We shall show how this condition may be used to find the distribution function for the gas particles in a state of statistical equilibrium.

The problem is to find $\overline{n}_j$ such that the

Sum

$S = \sum_j G_j \overline{n}_j \log\left(\frac{e}{\overline{n}_j}\right)$ has the maximum value possible under the subsidiary conditions.

$$\sum_j N_j = \sum_j G_j \overline{n}_j = N$$

$$\sum_j \varepsilon_j N_j = \sum_j \varepsilon_j G_j \overline{n}_j = E$$

which express the constancy of the total number of particles N and of total energy E of the gas.

Following the usual method of Lagrange's undetermined multipliers, we have to equate to zero the derivatives. $\frac{\partial}{\partial \bar{n}_j}\left(S+\alpha N+\beta E\right)=0$

where α *and* β are constants. Effecting the differentiation, one gets

$$\frac{\partial S}{\partial \bar{n}_j}+\alpha\frac{\partial}{\partial \bar{n}_j}\left(G_j\bar{n}_j\right)+\beta\frac{\partial}{\partial \bar{n}_j}\left(\varepsilon_j G_j\bar{n}_j\right)=0$$

Or $\quad G_j\left(-\log\bar{n}_j+\alpha+\beta\varepsilon_j\right)=0$

Hence, $\log\ \bar{n}_j=\alpha+\beta\varepsilon_j$

Or $\quad \bar{n}_j=e^{\alpha+\beta\varepsilon_j}$

The is just the Boltzmann distribution, the constants α and β being given in terms of T and μ by

$$\alpha=\frac{\mu}{T},\ \beta=-\frac{1}{k_B T}$$

17.6 Illustrative Examples

Example17.2 Explain Doppler broadening of spectral lines.

Sol. The radiation emitted by the molecules in a discharge tube is observed to have a finite width due to random motion of the molecules.

The transverse motion does not lead to Doppler broadening (provided v<<c, which is the case here). The wavelength of the light emitted by a molecule moving away from the observer with velocity v_x is given by

$\lambda=\lambda_0\left(1+\frac{v_x}{c}\right)$ Where λ_0 is the wavelength of the light emitted by a molecule at rest.

The intensity of the radiation emitted by molecules with velocity v_x to v_x+dv_x may be written as

$$I(\mathrm{v}_x)dv_x=\alpha N f(v_x)\,\mathrm{d}\,v_x$$

Where α is the radiation emitted per molecule.

Since $\lambda = \lambda_0\left(1+\frac{v_x}{c}\right)$, We have

$$v_x = c\left(\frac{\lambda-\lambda_0}{\lambda_0}\right);\ d\,v_x = \frac{cd\lambda}{\lambda_0}$$

Hence $I(\lambda)\mathrm{d}\lambda = \alpha N f(v_x)\left(\frac{dv_x}{d\lambda}\right)d\lambda$

$$= \alpha N\left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}}\exp\left[-\frac{mc^2}{2kT}\left(\frac{\lambda-\lambda_0}{\lambda_0}\right)^2\right]\frac{c}{\lambda_0}d\lambda$$

The intensity is a maximum at the unshifted wavelength (λ_0)and has a Gaussian shape.

17.7 Self learning Exercise-II

Q.1 Find the mean square width of the velocity distribution.

Q.2 Find the value of mean speed.

17.8 Summary

In this chapter we have deduced the Boltzmann's distribution of molecules of an ideal gas among various states by making use of Gibbs distribution formula. Ideal gas has been considered as a system of non interacting point particles of equal mass enclosed in a box with perfectly elastic walls. Applying the Gibbs distribution formula to the gas molecules, we have found that the probability that a molecule is in the k^{th} state is proportional to $e^{-\frac{\varepsilon_k}{k_BT}}$, and therefore the average number of molecules in that state denoted by $\overline{n}_k$ is given by

$$\overline{n}_k = ae^{-\frac{\varepsilon_k}{k_BT}}$$

where *a* is a constant given by the normalization condition :

$$\sum \overline{n}_k = N$$

We have also deduced the distribution formula for the number of molecules per unit volume with momenta in the given intervals dp_x, dp_y, dp_z (the Maxwellian distribution):

$$dN_{\vec{p}} = \frac{N}{V}\left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left[-\left(p_x^2 + p_y^2 + p_z^2\right)/2mk_B T\right] dp_x dp_y dp_z$$

We have also considered a gas in an external field, in which the potential energy of a molecule depends only on the coordinates of its centre of mass: $u = u(x, y, z)$, u is the potential energy.

The Maxwellian distribution for the velocities of the molecules remains unchanged while the distribution for the coordinates of the centre of mass is given by

$$dN_{\vec{r}} = n_0 e^{-u(x,y,x)/k_B T} dV$$

This formula gives the number of molecules in an element of volume $dV = dx\,dy\,dz$; the quantity

$n(\vec{r}) = n_0 e^{-u(x,y,z)/k_B T}$ is the number density of the particles. This is called Boltzmann's formula. Finally we deduce the Boltzmann distribution for ideal gases not in equilibrium. We conclude this chapter with some representative problems.

17.9 Glossary

Equilibrium : A state in which a process and its reverse are occurring at equal rates so that no overall change is taking place:

Gibbs : Josiah Willard Gibbs (February 11, 1839 – April 28, 1903) was an American scientist who made important theoretical contributions to physics, chemistry, and mathematics. His work on the applications of thermodynamics was instrumental in transforming physical chemistry into a rigorous deductive science. Together with James Clerk Maxwell and Ludwig Boltzmann, he created statistical mechanics (a term that he coined), explaining the laws of thermodynamics as consequences of the statistical properties of large ensembles of particles.

Discharge tube : A tube containing charged electrodes and filled with a gas in which ionization is induced by an electric field. The gas molecules emit light as they return to the ground state.

Quasi *:* used to show that something is almost, but not completely, the thing described

17.10 Answers to Self Learning Exercises

Answers to Self Learning Exercise-I

Ans.1: $\bar{\varepsilon} = \frac{1}{2}m\overline{v^2} = \frac{1}{2}m.\frac{3kT}{m} = \frac{3}{2}kT.$

Ans.2: $\frac{3kT}{m}$

Hint: $\overline{v_x^2} = \frac{\int_{-\infty}^{\infty} v_x^2 e^{-\frac{mv_x^2}{2kT}} dv_x}{\int_{-\infty}^{\infty} e^{-\frac{mv_x^2}{2kT}} dv_x} = \frac{kT}{m}$

$\therefore \overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2} = \frac{3kT}{m}$

Ans.3: Maxwellian distribution in terms of Cartesian coordinates in "Velocity space" is

$$dw_{\bar{v}} = \left[\frac{m}{2\pi k_B T}\right]^{\frac{3}{2}} e^{-m\left(v_x^2+v_y^2+v_z^2\right)/2k_BT} dv_x dv_y dv_z$$

Where T is expressed in energy units.

If we change from Cartesian spherical coordinates, the result is

$$dw_{\bar{v}} = \left[\frac{m}{2\pi k_B T}\right]^{\frac{3}{2}} e^{-mv^2/2k_BT} v^2 \sin\theta d\theta d\phi dv$$

Where v is the absolute magnitude of the velocity and θ and ϕ the polar angle and azimuthal angle which determine the direction of the velocity.

Answers to Self Learning Exercise-II

Ans.1: The width of the velocity distribution is given by

$$\overline{\left(v-\bar{v}\right)^2} = \overline{v^2} + (\bar{v})^2 - 2\overline{v\bar{v}}$$

$$= \overline{v^2} + (\bar{v})^2 = \overline{v^2} = \frac{3kT}{m}$$

Ans.2:

$$\bar{v} = \frac{\int_0^\infty v.v^2 e^{-\frac{mv^2}{2kT}} dv}{\int_0^\infty v^2 e^{-\frac{mv^2}{2kT}} dv} = \sqrt{\frac{8kT}{m\pi}}$$

The integral now runs only from zero to infinity since speed is a scalar quantity.

17.11 Exercise

Q.1 Find the mean square speed.

Q.2 Find on what ratio are $\sqrt{\overline{v^2}} : \bar{v} : v_{mostprobable}$.

Q.3 Find the Maxwellian distribution for velocities in cylindrical coordinates in velocity space.

Q.4 Find the probability distribution for the absolute magnitude of the velocity.

Q.5 Find the density of gas in a cylinder of radius R and length *l* rotating about its axis with angular velocity Ω, there being a total of N molecules in the cylinder.

Q.6 Find the number $d\upsilon_v$ of collisions of molecules per unit time (and per unit area of the wall surface), in which the velocity components are in given intervals dv_x, dv_y, dv_z.

Q.7 Find the number of impacts of gas molecules on unit area of the wall per unit time for which the angle between n the direction of the velocity of the molecule and the normal to the surface lies between θ and $\theta + d\theta$.

17.12 Answers to Exercise

Ans.1:

$$\overline{v^2} = \frac{\int_0^\infty v^4 e^{-\frac{mv^2}{2kT}} dv}{\int_0^\infty v^2 e^{-\frac{mv^2}{2kT}} dv} = \frac{3kT}{m}$$

Ans.2: 1.22 : 1.13 : 1

Ans.3: $dw_{\vec{v}} = \left[\frac{m}{2\pi k_B T}\right]^{\frac{3}{2}} e^{-\frac{m(v_z^2+v_r^2)}{2k_B T}} v_r dv_r dv_z d\phi$

Ans.4: $dw_v = 4\pi\left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2k_B T}} v^2 dv$

(Hint : Integrate with respect to angle θ and ϕ.

Ans.5: Rotation of a body as a whole is equivalent to the presence of an external field with potential energy $-\frac{1}{2}m\Omega^2 r^2$ (Where *r* is the distance from the axis of rotation) The gas density is therefore

$$n(r) = Ae^{m\Omega^2 r^2 / 2k_B T}$$

Normalization gives

$$n(r) = \frac{Nm\Omega^2 e^{m\Omega^2 r^2 / 2k_B T}}{2\pi k_B T\left(e^{m\Omega^2 r^2 / 2k_B T} - 1\right)}$$

Ans.6: We take an element of surface area of the vessel wall and define a coordinate system with the z-axis perpendicular to this element, which may then be written as dx dy.

Of the molecules in the gas, those which reach the vessel wall in unit time, i.e. collide with it, are just those whose z-coordinate does not exceed the component v_z of their velocity along that axis (which of course, must also be directed towards the wall, not away from it).

Therefore

$$d\upsilon_{\vec{v}} = \frac{N}{V}\left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(\frac{-m(\mathrm{v}_x^2 + \mathrm{v}_y^2 + \mathrm{v}_z^2)}{2k_B T}\right) v_z dv_x dv_y dv_z$$

From this we easily find the total number υ of impacts of gas molecules on unit area of the vessel wall per unit time. To do so we integrate over all velocities v_z from 0 to ∞ and over v_x and v_y from $-\infty$ to $+\infty$, integration

over v_z from $-\infty$ to 0 is not required, since $v_z < 0$ the molecule is travelling away from the wall and so does not collide with it Hence

$$\upsilon = \frac{N}{V}\sqrt{\frac{k_B T}{2\pi m}} = \frac{P}{\sqrt{2\pi m k_B T}}$$

Ans.7: $d\upsilon_\theta = \frac{N}{V}\left[\frac{2k_B T}{m\pi}\right]^{\frac{1}{2}} \sin\theta\cos\theta d\theta$

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UNIT-18
The Fermi Distribution

Structure of the Unit

18.0 Objectives

18.1 Introduction

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18.0 Objectives

(i) To obtain Fermi distribution

(ii) To discuss Fermi gas of elementary particles with special attention to degenerate electron gas

(iii) To describe specific heat of a degenerate electron gas.

18.1 Introduction

Statistical mechanics is useful to describe a system, composed of large

number of particles , as average effects of properties of particles without considering the properties of individual particles.

When the system consisting of indistinguishable, identical particles, its behavior can be determined by quantum statistical distribution. One of such distribution is Fermi (also known as Fermi-Dirac) distribution in which particles obey the Pauli Exclusion Principle; according to this no more than one particle can be in the same state. Such particles are called Fermions.

In this unit we will discuss Fermi distribution law and specific heat of a degenerate electron gas.

18.2 Fermi Distribution

Since Fermions obeys Pauli exclusion principal, hence occupancy of a state is either zero or one. So total number of available states must be greater than or equal to total number of particles.

Suppose there are n_j particles to be distributed among g_j states with energy E_j then first particle may be in any one of g_j states, second particle in $g_j - 1$ and so on, so, total occupancy of g_j states with n_j particle is gives as

$$g_j(g_j-1)(g_j-2).....(g_j-n_j+2)(g_j-n_j+1)$$

$$= \frac{g_j!}{(g_j-n_j)!}$$

Since all particles in this distribution are indistinguishable, hence total $n_j!$ combination belongs to same distribution.

Then number of distinguishable ways of occupation of levels is

$$\frac{g_j!}{(g_j-n_j)!n_j!}$$

Since number of available states with different energies are varies. Hence total number of distinguishable different ways of occupation of all levels with different energies is

$$\boxed{W = \prod_j \frac{g_j!}{(g_j-n_j)!n_j!}} \qquad (1)$$

Taking log on both sides, gives

$$\log w = \sum_j \left[\log \{g_i!\} - \log\{(g_i - n_j)!\} - \log\{n_j!\} \right] \tag{2}$$

Since, for any j, g_j and n_j are much greater than one, hence Sterling approximation gives

$$\log\{g_j!\} = g_j \log g_j - g_j \tag{3}$$

$$\log\{(g_j - n_j)!\} = (g_j - n_j) \log(g_j - n_j) - (g_j - n_j) \tag{4}$$

and

$$\log\{n_j!\} = n_j \log n_j - n_j \tag{5}$$

using equations (3), (4) and (5) in equation (2), gives

$$\log w = \sum_j \left[g_j \log g_j - g_j - (g_j - n_j)\log(g_j - n_j) + g_j - n_j - n_j \log n_j + n_j \right]$$

or $$\log w = \sum_j \left[g_j \log g_j - (g_j - n_j)\log(g_j - n_j) - n_j \log n_j \right]$$

The most probable distribution can be determined by maximization of log w.

Hence differentiating above relation and taken equal to zero, gives

$$d(\log w) = \sum_j \left[d n_j \log(g_j - n_j) + 1 - d n_j \log n_j - 1 \right] = 0$$

or $$\sum_j \left[\log(g_j - n_j) - \log n_j \right] d n_j = 0 \tag{6}$$

Since total number of particles remains constant, i.e.

$$\sum_j d n_j = 0 \tag{7}$$

and total energy of the system is remain invariant, i.e.

$$\sum_j E_j \, d n_j = 0 \tag{8}$$

Multiply equation (7) by $(-\alpha)$, (8) by $(-\beta)$ and then adding equation (6), (7) and (8) gives

$$\sum_j \left(\log(g_j - n_j) - \log n_j \right) d n_j - \alpha \sum_j d n_j - \beta \sum_j E_j \, d n_j = 0$$

or $$\sum_j \left[\log(g_j - n_j) - \log n_j - \alpha - \beta E_j \right] d n_j = 0$$

Since $d n_j$ are independent, hence for any j-value

$$\log\left(g_j - n_j\right) - log\, n_j - \alpha - \beta E_j = 0$$

$$\text{or} \quad \log\left(\frac{g_j - n_j}{n_j}\right) = \alpha + \beta E_j$$

$$\text{or} \quad \frac{g_j - n_j}{n_j} = \exp\left(\alpha + \beta E_j\right)$$

$$\text{or} \quad \frac{g_j}{n_j} - 1 = \exp\left(\alpha + \beta E_j\right)$$

$$\text{or} \quad \frac{g_j}{n_j} = 1 + \exp\left(\alpha + \beta E_j\right)$$

$$\text{or} \quad \boxed{n_j = \frac{g_j}{1 + \exp\left(\alpha + \beta E_j\right)}} \tag{9}$$

where α, β are given in terms of Fermi energy $'E'_{F'}$ Boltzmann constant 'k' absolute temperature 'T' of the system as

$$\alpha = -\frac{E_F}{kT}$$

$$\text{and} \quad \beta = \frac{1}{kT}$$

$$\text{Hence} \quad \boxed{n_j = \frac{g_j}{\exp\left[\frac{\left(E_j - E_F\right)}{kT}\right] + 1}} \tag{10}$$

This is the ***Fermi (or Fermi-Dirac) distribution function***.

In the limit $T \to 0$

$$\frac{n_j}{g_j} = \begin{cases} 1 \;\; for \;\; \varepsilon < \varepsilon_F \\ 0 \;\; for \;\; \varepsilon > \varepsilon_F \end{cases}$$

If $\varepsilon = \varepsilon_F$ then

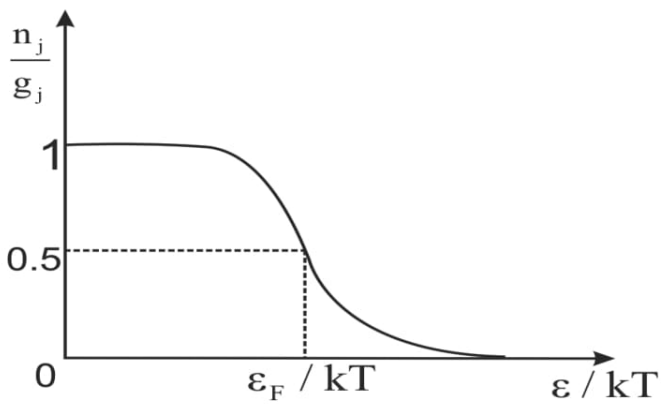
$$n_j = \frac{g_j}{1 + \exp\left(-\frac{\varepsilon_F}{kT} + \frac{\in_j}{kT}\right)}$$

$$n_j = \frac{g_j}{1+\exp\left(-\frac{\varepsilon_F}{kT}+\frac{\in_F}{kT}\right)}$$

$$n_j = \frac{g_j}{1+\exp(0)}$$

$$n_j = \frac{g_j}{2}$$

$$\boxed{For\ \varepsilon = \varepsilon_F\ , \frac{n_j}{g_j} = 0.5}$$



Thermodynamics of an ideal Fermi gas:

From eq. (2)

$$\log W = \sum_j \left[g_j \log g_j - \left(g_j - n_j\right)\log\left(g_j - n_j\right) - n_j \log n_j \right]$$

$$= \sum_j \left[g_j \log g_j - g_j \log\left(g_j - n_j\right) + n_j \log\left(g_j - n_j\right) - n_j \log n_j \right]$$

$$= \sum_j \left[-g_j \left\{ -\log g_j + \log\left(g_j - n_j\right)\right\} + n_j \left\{ -\log n_j + \log\left(g_j - n_j\right)\right\} \right]$$

$$= \sum_j \left[-g_j \left\{ \log\left(1 - \frac{n_j}{g_j}\right)\right\} + n_j \left\{ \log\left(\frac{g_j}{n_j} - 1\right)\right\} \right]$$

$$= \sum_j \left[n_j \log\left(\frac{g_j}{n_j} - 1\right) - g_j \log\left(1 - \frac{n_j}{g_j}\right) \right] \qquad (11)$$

From eq. (9)

$$n_j = \frac{g_j}{1+\exp\left(\alpha+\beta\in_j\right)}$$

$$\text{or} \quad \frac{n_j}{g_j} = \left[1+\exp\left(\alpha+\beta\in_j\right)\right]^{-1}$$

Hence from eq. (11)

$$\log W = \sum_j \left[n_j\left(\alpha+\beta\in_j\right) - g_j \log\left\{1-\frac{1}{1+\exp\left(\alpha+\beta\in_j\right)}\right\}\right]$$

$$= \sum_j \left[n_j\left(\alpha+\beta\in_j\right) - g_j \log\left\{\frac{1+\exp\left(\alpha+\beta\in_j\right)-1}{1+\exp\left(\alpha+\beta\in_j\right)}\right\}\right]$$

$$= \sum_j \left[n_j\left(\alpha+\beta\in_j\right) - g_j \log\left\{\frac{1}{1+\exp\left(-\alpha-\beta\in_j\right)}\right\}\right]$$

$$= \sum_j \left[n_j\left(\alpha+\beta\in_j\right) + g_j \log\left\{1+\exp\left(-\alpha-\beta\in_j\right)\right\}\right] \qquad (12)$$

Hence entropy of the system

$$\boxed{S = k\log W}$$

$$\Rightarrow \frac{S}{k} = \log W$$

From eq.(12)

$$\frac{S}{k} = \sum_j \left[n_j\left(\alpha+\beta\in_j\right) + g_j \log\left\{1+\exp\left(-\alpha-\beta\in_j\right)\right\}\right]$$

$$\frac{S}{k} - \alpha\sum_j n_j - \beta\sum_j n_j\varepsilon_j = \sum_j g_j \log\left[1+\exp\left(-\alpha-\beta\in_j\right)\right]$$

Here total number of particles $\sum_j n_j = N$ and

total energy of the system is

$$\sum_j E_j\, n_j = E$$

$$\frac{S}{k}-\alpha N-\beta E=\sum_j g_j \log\left[1+\exp\left(-\alpha-\beta \in_j\right)\right]$$

Since

$$\alpha=-\frac{\varepsilon_F}{kT},\ \beta=\frac{1}{kT}$$

$$n_j=\frac{g_j}{1+\exp\left(-\frac{\varepsilon_F}{kT}+\frac{\in_j}{kT}\right)}$$

Hence

$$\frac{S}{k}+\frac{N\varepsilon_F}{kT}-\frac{E}{kT}=\frac{N\varepsilon_F+ST-E}{kT}$$

$$\Rightarrow \frac{S}{k}+\frac{N\varepsilon_F}{kT}-\frac{E}{kT}=\frac{N\varepsilon_F-(\mathrm{E}-\mathrm{TS})}{kT}$$

$$=\frac{N\varepsilon_F-(\mathrm{E}-\mathrm{TS})}{kT}$$

$$=\frac{PV}{kT}$$

$$\Rightarrow \frac{PV}{kT}=\sum_j g_j \log\left[1+\exp\left(-\alpha-\beta \in_j\right)\right]$$

This equation shows thermodynamics behavior of the Fermi gas.

18.3 Self-Learning Exercise-I

Q.1 Is behavior of system of indistinguishable particles can be explained on the basis of quantum statistics?

Q.2 What are Fermions?

Q.3 What is Pauli exclusion principal?

Q.4 What do you understand by indistinguishable particles?

Q.5 What is Sterling approximation?

18.4 Fermi Gas of Elementary Particles

A system consisting of large number of elementary particles, which obey

A system consisting of large number of elementary particles, which obey Fermi-Dirac statistics, can be analyzed by assuming this system as an ideal gas of elementary particles known as Fermi gas.

Since a gas can be completely described by specified the position and momentum of each particle present in the gas.

Position and momentum of each particle can be specified in terms of three dimensional co-ordinates $x, y,\ z$ and momentum components $p_x,\ p_y,\ p_z$ respectively.

When six co-ordinates $x,\ y,\ z,\ p_x,\ p_y,\ p_z$ of each particles specified then the state of gas can be determined in phase space.

The phase space assumed to be made up by small phase cells having dimension as $\Delta x,\ \Delta y,\ \Delta z,\ \Delta p_x,\ \Delta p_y,\ \Delta p_z$ so, volume of each cell is equal to

$$\Delta x.\Delta y.\Delta z.\Delta p_x.\Delta p_y.\Delta p_z$$

According to Heisenberg uncertainty principal, position and momentum components are related as

$$\Delta x.\Delta p_x \cong h$$

$$\Delta y.\Delta p_y \cong h$$

$$\Delta z.\Delta p_z \cong h$$

So minimum volume of cell is

$$\Delta x.\Delta y.\Delta z.\Delta p_x.\Delta p_y.\Delta p_z = h^3$$

Consider a Fermi gas of volume V, with particle has a momentum between p and $p+dp$, then number of states is given as

$$g(p)dp = \frac{1}{h^3}(\Delta x\,\Delta y\,\Delta z)(\Delta p_x\,\Delta p_y\,\Delta p_z)$$

If differences are small enough, then

$$\boxed{g(p)dp = \frac{V}{h^3}.4\pi\, p^2 dp} \qquad (13)$$

Since energy of particle is given as

$$E = \frac{p^2}{2m}$$

$$\Rightarrow \qquad p^2 = 2mE \tag{14}$$

$$\Rightarrow \qquad p = (2mE)^{1/2}$$

$$\text{and} \qquad dp = (2m)^{1/2} \frac{dE}{2E^{1/2}} \tag{15}$$

From equation (13), having values of equations (14) & (15)

$$g(E)dE = \frac{V}{h^3} 4\pi . 2mE . (2m)^{1/2} \frac{dE}{2E^{1/2}}$$

$$\left.\begin{aligned} \Rightarrow \qquad g(E)dE &= \frac{V}{h^3} 4\pi \left(2m^3\right)^{1/2} E^{1/2} dE \\ \Rightarrow \qquad g(E) &= \frac{4\pi V \left(2m^3\right)^{1/2} E^{1/2}}{h^3} \end{aligned}\right\} \tag{16}$$

Hence this equation gives number of states between energy E and $E + dE$

18.5 A Degenerate Electron Gas

Outer most electrons in metals are distributed among different levels in conduction band following the exclusion principle. Zero level of this band is taken at the lowest level of conduction band. These electrons in conduction band form a degenerate Fermi gas. Since the energy of electrons in the conduction band is continuous, hence number of energy levels g_j in Fermi-Dirac distribution function replaced by continuous value $g(E)dE$.

Here $g(E)dE$ is given by (equation (16)

$$g(E)dE = \frac{4\pi V \left(2m^3\right)^{1/2} E^{1/2}}{h^3} dE$$

Since maximum two electrons with opposite spin are filled in same energy level, so effective number of states between energy E and $E + dE$ is

$$g(E)dE = \frac{8\pi V \left(2m^3\right)^{1/2} E^{1/2}}{h^3} dE \tag{17}$$

The Fermi Dirac distribution for continuous system is (from equation (9))

$$dn = \frac{g(E)dE}{1 + \exp\left[(E - E_F)/k.T\right]}$$

Hence number of electrons have energy between E and $E+dE$ is given as (using equation (17)

$$dn = \frac{8\pi V\left(2m^3\right)^{1/2} E^{1/2}\, dE}{h^3\left[1+\exp\left[E-E_F/k.T\right]\right]} \tag{18}$$

$$\left(\frac{dn}{dE}\right) = \frac{8\pi V\left(2m^3\right)^{1/2} E^{1/2}}{h^3\left[1+\exp\left\{E-E_F/k.T\right\}\right]}$$

At T = 0K (absolute zero) If $E > E_F$,

then $\frac{dn}{dE} = 0$ and for $E \le E_F$,

then $\frac{dn}{dE} = \frac{8\pi V\left(2m^3\right)^{1/2} E^{1/2}}{h^3}$

$$\Rightarrow \quad \int_0^N dn = \frac{8\pi V\left(2m^3\right)^{1/2}\int_0^{E_F} E^{1/2}dE}{h^3}$$

$$\Rightarrow \quad N = \frac{8\pi V\left(2m^3\right)^{1/2}}{h^3}\frac{2}{3}E_F^{3/2}$$

$$\Rightarrow \quad E_F^{3/2} = \left(\frac{3N h^3}{16\pi V\left(2m^3\right)^{1/2}}\right)$$

$$\Rightarrow \quad E_F = \left[\frac{3h^3}{16\pi\left(2m^3\right)^{1/2}}\left(\frac{N}{V}\right)\right]^{2/3}$$

$$\Rightarrow \quad \boxed{E_F = \frac{h^2}{8m}\left(\frac{3N}{\pi V}\right)^{2/3}} \tag{19}$$

Hence all the levels with energy less then E_F ***(known as Fermi energy) are filled at absolute zero***. If number of free electrons per unit volume $\left(\frac{N}{V}\right)$ is known, the Fermi energy of a metal can be determined by equation (19).

White Dwarf Star

White dwarf star is so hot that to first approximation all the atoms are fully ionized. The matter responsible for mass of white dwarf is mainly ${}_2He^4$ while the electrons provide charge neutrality and supply pressure that keeps the star from collapsing under its own pressure. The electrons are Fermions, so they fill up all the available levels to the Fermi energy and create pressure to prevent white dwarf from collapsing.

18.6 Specific Heat of a Degenerate Electron Gas

Since all the levels up to Fermi energy E_F are filled up at absolute zero temperature.

When temperature is raised from o to T K, then only small fraction of electrons centered around Fermi energy E_F are absorb energy of the order of kT and excited to upper unfilled levels. Other electrons cannot be acquiring energy because levels to which electrons would be excited are already filled.

Hence number of excited electrons is (from equation (18))

$$N_{ex} \sim \frac{8\pi V}{h^3}\left(2m^3\right)^{1/2}.E_F^{1/2}.kT \qquad \text{From equation (19)}$$

$$N_{ex} \sim .\frac{3N}{2E_F^{3/2}}.E_F^{1/2}.kT$$

$$\text{or} \qquad N_{ex} \sim \frac{3NKT}{2E_F}$$

Let $E_F = kT_F$ { T_F is known as Fermi temperature}

$$\text{Hence } N_{ex} \sim \frac{3N}{2}\left(\frac{T}{T_F}\right) \qquad (20)$$

Since average excitation energy per electron is kT, so increase in energy when temperature raised from 0 to T K is

$$E = N_{ex}.kT$$

$$= \frac{3N}{2}\left(\frac{T}{T_F}\right)kT. \qquad \{\text{from equation (20)}\}$$

$$E = \frac{3NkT^2}{2T_F}$$

Hence electronic heat capacity is

$$C_{el} = \frac{dE}{dT} = 3Nk\left(\frac{T}{T_F}\right)$$

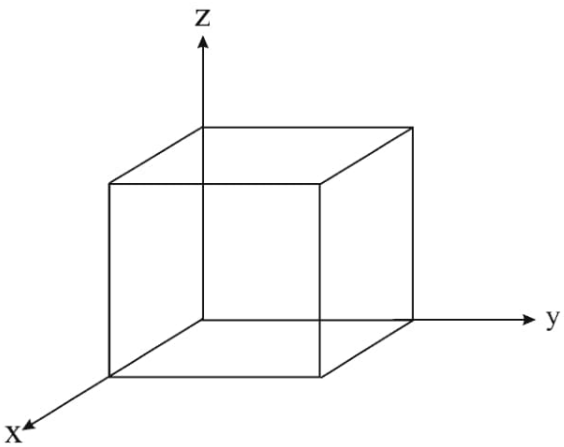
Hence ***electronic heat capacity of metals is proportional to absolute temperature***.

18.7 Thermionic Emission (Richardson effect)

An example of degenerate electron gas is the thermionic emission of electrons from metallic surface.

Electrons in conduction band of metals are treated as free and remain there until a specific energy is supplied to these electrons. This specific energy, known as work function of metal ,which depends on the nature of metal, temperature of surface of metal etc.

In thermionic emission, the metallic filament is heated, so that electrons in filaments acquire sufficient energy to overcome the surface.



Let us consider a metallic surface parallel to xy plane and at temperature T Kelvin. Let ε be the energy of electrons having momentum p_x, p_y, p_z and velocity v_x, v_y, v_z along x, y, z axis respectively.

The number of electron states having momentum below p_x and $p_x + dp_x, p_y$ and $p_y + dp_y$, p_z and $p_z + dp_z$ is

$$g(p)dp = \frac{2V}{h^3} dp_x dp_y dp_z$$

where factor 2 shows the fact that each state is filled with maximum two electrons of opposite spins.

Hence the number density in Fermi-Dirac distribution for continuous system is given by

$$dn' = \frac{g(p)dp}{V\left[1+exp\left(\frac{\varepsilon - E_F}{kT}\right)\right]}$$

$$= \frac{2}{h^3} \frac{dp_x dp_y dp_z}{\left[1+exp\left(\frac{\varepsilon - E_F}{kT}\right)\right]}$$

The differential current density due to emitting electrons along a z direction is

$$dJ_z = ev_z dn'$$

or

$$= dJ_z = \frac{2e}{h^3} \frac{v_z dp_x dp_y dp_z}{\left[1+exp\left(\frac{\varepsilon - E_F}{kT}\right)\right]}$$

Since $v_z = \frac{p_z}{m}$, we have

$$dJ_z = \frac{2e}{mh^3} \frac{dp_x\ dp_y\ p_z dp_z}{\left[1+exp\left(\frac{\varepsilon - E_F}{kT}\right)\right]}$$

So total current density

$$J_Z = \frac{2e}{mh^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{p_z}^{+\infty} \frac{dp_x dp_y p_z dp_z}{\left[1+exp\left(\frac{\varepsilon - E_F}{kT}\right)\right]}$$

Here p_z is the momentum equivalent of work function.

Since supplied thermal energy is much greater then kT i.e.

$$(\varepsilon - E_F) \gg kT$$

Here

$$J_z = \frac{2e}{mh^3}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{p_z}^{+\infty} exp\left(-\frac{\left(\varepsilon - E_F\right)}{kT}\right).dp_x dp_y p_z dp_z$$

Or $$J_z = \frac{2e}{mh^3}\exp\left(\frac{E_F}{kT}\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{p_z}^{+\infty}\exp\left(-\frac{\varepsilon}{kT}\right)dp_x dp_y p_z dp_z$$

Since total energy is

$$E = \frac{p_x^2 + p_y^2 + p_z^2}{2m}$$

Hence $$J_z = \frac{2e}{mh^3}\exp\left(\frac{E_F}{kT}\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{p_z}^{+\infty}\left[\exp\left[-\left(\frac{p_x^2 + p_y^2 + p_z^2}{2mkT}\right)\right]\right]dp_x dp_y p_z dp_z$$

$$J_z = \frac{2e}{mh^3}\exp\left(\frac{E_F}{kT}\right)\int_{-\infty}^{+\infty}\left[\exp\left(-\frac{p_x^2}{2mkT}\right)\right]dp_x\int_{-\infty}^{+\infty}\left[\exp\left(-\frac{p_y^2}{2mkT}\right)\right]dp_y \int_{p_z}^{+\infty}\left[\exp\left(-\frac{p_z^2}{2mkT}\right)\right]p_z dp_z$$

Using standard integral

$$\int_{-\infty}^{+\infty}\exp\left(-bx^2\right)dx = \sqrt{\frac{\pi}{b}}$$

Current density is given by

$$J_z = \frac{2e}{mh^3}\exp\left(\frac{E_F}{kT}\right)\left[\sqrt{2m\pi kT}\right]\left[\sqrt{2m\pi kT}\right]\int_{p_z}^{\infty}\left[\exp\left(-\frac{p_z^2}{2mkT}\right)\right]p_z dp_z$$

$$= \frac{4e\pi kT}{h^3}\exp\left(\frac{E_F}{kT}\right)\int_{\left(\frac{p_z^2}{2mkT}\right)}^{\infty}\left[\exp\left(-\frac{p_z^2}{2mkT}\right)\right].\left[d\left(-\frac{p_z^2}{2mkT}\right)\right].\left[-mkT\right]$$

$$= \frac{4\pi\, ekT}{h^3}\exp\left(\frac{E_F}{kT}\right)\left[-mkT\right]\left[\exp\left[-\frac{p_z^2}{2mkT}\right]\right]_{\frac{p_z^2}{2mkT}}^{\infty}$$

$$= \frac{4\pi\, mek^2T^2}{h^3}\exp\left(\frac{E_F}{kT}\right).\exp\left(-\frac{p_z^2}{2mkT}\right)$$

Since $\varepsilon_p = \frac{p_z^2}{2mkT}$ is the minimum required energy to leave the metallic surface.

So $$J_z = \frac{4\pi\, mek^2}{h^3}T^2 exp\left(-\frac{\left(\varepsilon_p - E_F\right)}{kT}\right)$$

Since $\varepsilon_p - E_F = e\phi$

Where ϕ is work function of the metal

Hence $J_z = \frac{4\pi mek^2}{h^3} T^2 \left[\exp\left(-\frac{e\phi}{kT} \right) \right]$

Taking $\frac{4\pi mek^2}{h^3} = A$ and $\frac{e\phi}{k} = b$

The relation is $\boxed{J_z = A\,T^2 \left[\exp\left(-\frac{b}{T} \right) \right]}$

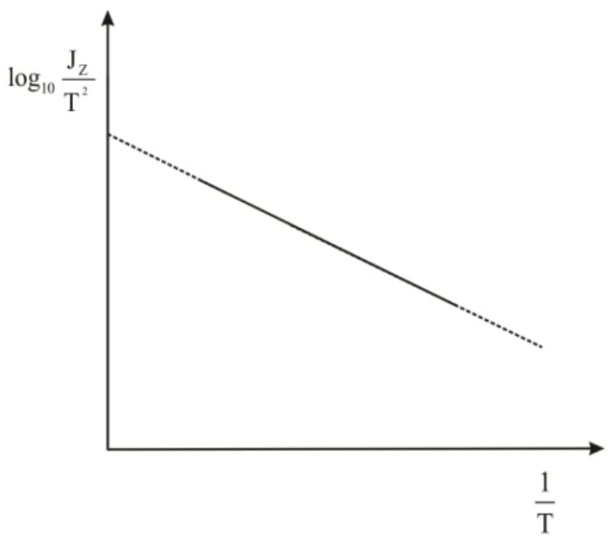
which is ***Richardson's equation or Richardson-Dushman equation***.

Taking log on both side.

$$\log_{10}\left(\frac{J_z}{T^2}\right) = \log_{10}\left[A \exp\left(-\frac{b}{T} \right) \right]$$

Or $$\log_{10}\left(\frac{J_z}{T^2}\right) = \log_{10} A - 0.434b.\frac{1}{T}$$

If we plot $\log_{10}\left(\frac{J_z}{T^2}\right)$ against $\frac{1}{T}$,then we get a straight line with slope $(-0.434b)$ and an intercept $\log_{10} A$ on $\log_{10}\left(\frac{J_z}{T^2}\right)$ axis.



The slope of the plot gives an estimate of the work function of the metal

18.8 Self-Learning Exercise-II

Q.1 How many dimensions phase space has?

Q.2 Write Heisenberg's uncertainly principle for x-coordinates

Q.3 What is a Fermi gas?

Q.4 What do you mean by 'degeneracy'?

Q.5 What is conduction band?

18.9 Summary

Electrons are the fermions that obey Fermi-Dirac statistics. Fermi-Dirac distribution function and number of states for electrons are derived in this unit and heat capacity of electrons in metals has discussed.

18.10 Glossary

***Fermions*:** Elementary Particles that obey Fermi-Dirac Statistics

***Degenerate gas*:** when particles of a gas with different quantum number has the same energy states then this the gas is termed as degenerate gas

***Phase Space*:** Six dimensional space related to momentum and coordinates of particles

***Conduction Band*:** Outer most band responsible for conduction of electricity in metals.

***Fermi energy*:** If all the levels with energy less than a 'specific energy' are filled at absolute zero, then this 'specific energy' is the Fermi energy

***Fermi gas*:** A gas consisting of large number of elementary particles, which obey Fermi-Dirac statistics

18.11 Answers to Self Learning Exercises

Answers to Self Learning Exercise-I

Ans.1: Yes

Ans.2: Particles that obey Fermi-Dirac Statistics.

Answers to Self Learning Exercise-II

Ans.1: Six

Ans.2: $\Delta x . \Delta p_x \cong h$

18.12 Exercise

Section-A (Very Short Answer Type)

Q.1 Give examples of Fermions.

Q.2 What are the values of occupancy of Fermi levels?

Q.3 What is the minimum volume of phase cell?

Q.4 In what condition quantum statistics reduces to classical statistics?

Q.5 What is Fermi temperature?

Q.6 Write lowest value of absolute temperature scale?

Q.7 What is the unit of absolute temperature?

Q.8 What is Fermi energy?

Q.9 Why only a small fraction of electrons acquire energy at higher temperature?

Q.10 Define heat capacity.

Section-B: Short Answer Type Questions

Q.11 Explain phase space?

Q.12 What do you mean by electron gas?

Q.13 Explain degenerate energy state.

Q.14 Discuss Fermi energy of a metal.

Q.15 What is mean by Fermi level?

Q.16 Determine the Fermi Energy of electrons in Copper having one electron per atom.

Given-

Avogadro number – $6x10^{23}$ atoms/ Mole

Atomic weight of Copper – 0.0635 Kg/ Mole

Density of Copper – 8.94 gm/ c.c.

Planck's constant – $6.62x10^{-34}$ J.Sec

Mass of electron – 9.1×10^{-31} Kg

Boltzmann constant – 1.38×10^{-23} J/ K

Section-C: Long Answer Type Questions

Q.17 Describe degenerate electron gas and obtain number of states of energy between E and $E + dE$. .

Q.18 Discuss Fermi-Dirac distribution function for electron gas

Q.19 Derive specific heat capacity of electron gas.

Q.20 Derive Fermi-Dirac distribution function

18.13 Answers to Exercise

Ans.1: Electrons, Positron, Proton.

Ans.2: Either 0 or 1.

Ans.3: h^3, where h is Planck's constants.

Ans.4: At high temperature.

Ans.5: Ratio of Fermi energy and Boltzmann constant.

Ans.6: Zero

Ans.7: K (Kelvin)

Ans.16: Since density of Copper- 8.94×10^{-3} Kg/ 10^{-6} m^3

$= 8.94 \times 10^{3}$ Kg/m^3

and volume= atomic weight/density= $0.0635/(8.94 \times 10^{3})$

$= 635 \times 10^{-4} / 8940$

$= 7.1 \times 10^{-6}$ m^3

Now electron density(N/V) = Avogadro number/volume

$= 6.02 \times 10^{23} / 7.1 \times 10^{-6}$

$= (602/71) \times 10^{28}$

$= 8.48 \times 10^{28}$ atoms/m^3

So, Fermi energy of Copper = $E_F = h^2/8m\ (3N/\pi V)^{2/3}$

$= ((6.62 \times 10^{-34})^2/8 \times 9.1 \times 10^{-31}) \times (3 \times 8.48 \times 10^{28}/3.14)^{2/3}$

$=11.27 \times 10^{-19}$ Joule

$=11.27 \times 10^{-19} / 1.6 \times 10^{-19}$ eV

$=7.04$ eV

References and Suggested Readings

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UNIT-19
The Bose Distribution

Structure of the Unit

19.0 Objectives

19.1 Introduction

19.2 The Bose distribution

19.3 Bose gas not in equilibrium

19.4 Bose gas of elementary particles

19.5 A degenerate Bose gas

19.6 Self learning exercise I

19.7 Black body radiation

19.8 Self learning exercise II

19.9 Summary

19.10 Glossary

19.11 Answer to self learning exercises

19.12 Exercise

References and Suggested Readings

19.0 Objectives

After interacting with the material presented here students will be able to understand

- The Bose distribution,
- Thermodynamics of free quantum
- Bose-Einstein condensation
- Black body radiation
- Plank's distribution formula

19.1 Introduction

We shall now investigate in detail the physical behavior of a class of systems in which, while the intermolecular interactions are still negligible, the effects of quantum statistics assume an increasingly important role. This means that the temperature T and the particle density n of the system no longer conform to the criterion

$$n\lambda^3 \equiv \frac{nh^3}{(2\pi mkT)^{\frac{3}{2}}} \ll 1$$

where λ is the mean thermal wavelength or thermal de Broglie wavelength of the particles. When $n\lambda^3$ is of the order of unity, then not only does the behavior of a system exhibit significant departure from typical classical behavior but it is also influenced by whether the particles constituting the system obey Bose–Einstein statistics or Fermi–Dirac statistics. Under these circumstances, the properties of the two kinds of systems are themselves very different. In the present chapter we consider systems belonging to the first .

Bose-Einstein distribution (B–E statistics) was introduced for ***photons*** in 1924 by Bose and generalized to atoms by Einstein in 1924-25. B-E statistics determines the statistical distribution of identical indistinguishable bosons over the energy states in thermal equilibrium. ***Bosons, unlike fermions, are not subject to the Pauli Exclusion Principle: an unlimited number of particles may occupy the same state at the same time***. This explains why, at low temperatures, bosons can behave very differently from fermions; all the particles will tend to congregate at the same lowest-energy state, forming what is known as a Bose–Einstein condensate.

19.2 The Bose distribution

Bosons are essentially different from fermions as there is no limitation on the the occupancy of an orbital. We want to find the distribution function for bosons as we did for fermions. This time consider a system of noninteracting bosons in thermal and diffusive contact with a reservoir. Let ε be the energy of an orbital when it is occupied by one boson. Thus, when the occupancy is N, the

energy will be nε. As before, we treat one orbital as the system, the rest as part of the reservoir. The number of particles in the single orbital is arbitrary.

$$Z = \sum_{N,r} e^{\beta(N\mu - E_{(N,r)})}$$

for all states and occupancies of the orbital. This time we write

$$Z = 1 + e^{\beta(\mu-\varepsilon)} + e^{2\beta(\mu-\varepsilon)} + \cdots$$

$$= 1 + e^{\beta(\mu-\varepsilon)} + e^{\beta(\mu-\varepsilon)^2} + \cdots.$$

We can rewrite this as

$$Z = \sum_{N=0}^{\infty} e^{N\beta(\mu-\varepsilon)}$$

The upper limit on N should be the number of particles in the combined system and reservoir. Since the reservoir can be as large as we like, we will let the sum run to ∞ to enable the series to be conveniently summed.

If we let x = $e^{\beta(\mu-\varepsilon)}$, then we have a geometric series

$$Z = \sum_{N=0}^{\infty} x^N = \frac{1}{1-x} = \frac{1}{1-e^{\beta(\mu-\varepsilon)}}$$

This summation is possible provided that $e^{\beta(\mu-\varepsilon)} < 1$. This will be true in all applications since if it were not the number of bosons in the system would not be bounded.

Now that we have the grand partition function, we can determine the average occupancy. Thus the average occupancy of an orbital is

$$< N > = \sum_{N,r} N p_{N_r}$$

Since we are taking care of the sum over states by writing Nε, we can replace this by a sum over N. Thus, we write

$$< N > = \sum_{N} N p_N = 0.p_0 + 1.p_1 + 2.p_2 + \cdots$$

Thus we need to evaluate

$$< N >= \sum_N \frac{Ne^{N\beta(\mu-\varepsilon)}}{Z} = \sum_N \frac{Ne^{-N\beta(\varepsilon-\mu)}}{Z}$$

To evaluate this let x = $\beta(\varepsilon - \mu)$, then we can write

$$< N >= \sum_N \frac{Ne^{-Nx}}{Z}$$

We can see that this can be easily rewritten as

$$< N >= -\frac{1}{Z}\sum_N \frac{\partial}{\partial x} e^{-Nx} = -\frac{1}{Z}\frac{\partial Z}{\partial x}$$

Now we can evaluate this expression

$$< N >= -(1-e^{-x})\frac{\partial}{\partial x}(1-e^{-x})^{-1} = (1-e^{-x})(1-e^{-x})^{-2}e^{-x}$$
$$= \frac{e^{-x}}{1-e^{-x}} = \frac{1}{e^{x}-1}$$

$$\boxed{\langle N \rangle = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}}$$

This is the Bose-Einstein distribution. As we'll see the switch from +1 to −1 has large physical consequences.

We will sometimes write Bose-Einstein distribution as

$$< N_i >= \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$

19.3 Bose Gas not in Equilibrium

For Bose statistics, each quantum state may contain any number of particles, so that the statistical weight $\Delta\Gamma_i$ is the total number of ways of distributing N_i particles among G_i states.

$$\Delta\Gamma_i = \frac{(G_i + N_i - 1)!}{(G_i - 1)!\, N_i!}$$

Taking the logarithm of above expression and neglecting unity in comparison with the large number G_i+N_i and G_i,

$$S = \sum_i \{(G_i + N_i)\log(G_i + N_i) - N_i \log N_i - G_i \log G_i\}$$

In terms of the number $\bar{n}_\iota$ we can write the entropy of a Bose gas not in equilibrium as

$$S = \sum_i G_i\{(1+\bar{n}_\iota)\log(1+\bar{n}_\iota) - \bar{n}_\iota \log \bar{n}_\iota\}$$

It is easily seen that that the condition for this expression to be a maximum in fact givers the Bose distribution.

Above expression tend to the Boltzmann formula at $n_i \ll g_i$ since

$$G_i! \approx (G_i - n_i)!\, G_i^{n_i}, (G_i + n_i - 1)! \approx (G_i - 1)!\, G_i^{n_i}$$

At $n_i \ll g_i$.

Finally, let us specify the expression for the entropy of Bose gas at $n_i \gg 1$ since we will need this expression later to discuss the Bose condensation. We have

$$\Delta\Gamma_i \approx \frac{n_i^{g_i-1}}{(g_i-1)!}$$

and

$$S = \sum_i G_i \ln(en_i)$$

19.4 Bose Gas of Elementary Particles

Let's consider a gas consisting of elementary particles. The energy of an elementary particle is just the kinetic energy of its translational motion, which is always quasi classical

We therefore have

$$\varepsilon = (p_x^2 + p_y^2 + p_z^2)/2m$$

The number of particles in a volume element in the phase space is found by multiplying the distribution by

$$gd\tau = \frac{g dp_x dp_y dp_z dV}{(2\pi\hbar)^3}$$

Where g=2s+1 (s, spin of the particles)

$$dN = \frac{gd\tau}{e^{\beta(\varepsilon-\mu)} - 1}$$

Integrating over V, we find the distribution for the components of the particle momentum; we find the distribution for the absolute magnitude of the momentum

$$dN_p = \frac{gVp^2dp}{2\pi^2\hbar^3(e^{\beta(\varepsilon-\mu)}-1)}$$

Where $\varepsilon = \frac{p^2}{2m}$, or the energy distribution

$$dN_\varepsilon = \frac{gVm^{\frac{3}{2}}\sqrt{\varepsilon}d\varepsilon}{2^{\frac{1}{2}}\pi^2\hbar^3(e^{\beta(\varepsilon-\mu)}-1)}$$

Integrating with respect to Ɛ, we obtain the total number of particles in the gas

$$N = \frac{gVm^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{\varepsilon}d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$

Now $z = \varepsilon/T$

$$\frac{N}{V} = \frac{g(mT)^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{z}dz}{e^{(z-\mu/T)}-1}$$

This formula implicitly determines the chemical potential of the gas as a function of its temperature and density.

Now the potential

$$\Omega = \frac{VgT(m)^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \sqrt{\varepsilon}d\varepsilon \log(e^{\beta(\varepsilon-\mu)}-1)$$

$$\Omega = -\frac{2}{3}\frac{Vg(m)^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \varepsilon^{\frac{3}{2}}d\varepsilon\ 1/(e^{\beta(\varepsilon-\mu)}-1)$$

The total energy of the gas

$$E = \int_0^\infty \varepsilon dN_\varepsilon = \frac{gVm^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \frac{\varepsilon^{\frac{3}{2}}d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$

Since $\Omega = -PV$, we therefore have

$$PV = \frac{2}{3}E$$

Now after substituting $z = \varepsilon/T$ in Ω, we obtain

$$\Omega = -PV = VT^{\frac{5}{2}}f(\mu/T)$$

Where f is a function of a single variable, i.e. Ω/Vis a homogeneous function of order 5/2 in μ and T.

$$\frac{S}{V} = -\frac{1}{V}\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu}$$

And

$$\frac{N}{V} = -\frac{1}{V}\left(\frac{\partial \Omega}{\partial T}\right)_{T,V}$$

Are homogeneous function of order 3/2 in μ and T, hence $\frac{S}{N} = \phi\left(\frac{\mu}{T}\right)$. Hence we see that in adiabatic process the ratio μ/T remains constant and $N/(V\,T^{3/2})$ is also a function of μ/T, only we have

$$\boxed{VT^{\frac{3}{2}} = constant}$$

Then

$$\boxed{PV^{\frac{5}{3}} = constant}$$

and also

$$T^{\frac{5}{2}}P = constant$$

The exponents, however, have nothing to do with the ratio of specific heats, $\frac{c_V}{c_P}$, since the conditions $\frac{C_P}{C_V} = \frac{5}{3}$ and $c_P - c_V = 1$ do not hold any more.

These equations are same as that of the poission adiabatic for an ordinary monatomic gas.

$$P = \frac{g2^{\frac{1}{2}}m^{\frac{3}{2}}T^{\frac{5}{2}}}{3\pi^2\hbar^3}\int_0^\infty \frac{z^{\frac{3}{2}}dz}{e^{(z-\mu/T)}-1}$$

In the limiting case of a Boltzmann gas ($e^{\frac{\mu}{T}} \ll 1$) these formula give Clapeyron's equation

Then

$$\int_0^\infty \frac{z^{\frac{3}{2}}dz}{e^{(z-\mu/T)}-1} \cong \int_0^\infty z^{\frac{3}{2}}e^{\left(\frac{\mu}{T}-z\right)}\left(1+e^{\left(\frac{\mu}{T}-z\right)}\right)dz = \frac{3}{4}\sqrt{\pi}\,e^{\frac{\mu}{T}}\left(1+\frac{1}{2^{\frac{5}{2}}}e^{\frac{\mu}{T}}\right)$$

$$\Omega = -PV = -\frac{gVm^{\frac{3}{2}}T^{\frac{5}{2}}}{(2\pi)^{\frac{3}{2}}\hbar^3}e^{\frac{\mu}{T}}\left(1+\frac{1}{2^{\frac{5}{2}}}e^{\frac{\mu}{T}}\right)$$

The first term in this expression represent Boltzmann value of the chemical potential of a monatomic gas. The next term gives the required corrections, so that we can write

$$\Omega = \Omega_{Boltz} - \frac{gVm^{\frac{3}{2}}T^{\frac{5}{2}}}{16(\pi)^{\frac{3}{2}}\hbar^3} e^{\frac{2\mu}{T}}$$

We also obtain corrections to the free energy

$$\mathrm{F} = F_{Boltz} - \frac{\pi^{\frac{3}{2}}N^2\hbar^3}{2gVT^{\frac{1}{2}}m^{\frac{3}{2}}}$$

Finally differentiating with respect to volume, we obtain

$$\mathrm{PV} = NT\left[1 - \frac{\pi^{\frac{3}{2}}N\hbar^3}{2gVT^{\frac{3}{2}}m^{\frac{3}{2}}}\right]$$

We see that the deviation of an ideal gas from classical properties, occurring when the temperature is lowered at constant density (degenerate). The value of gas pressure changes in the opposite direction, becoming less than the classical value, and hence we can say that here there is an effective attraction between the particles.

19.5 A Degenerate Bose Gas

The chemical potential of bosons is negative. It is given by the equation

$$\frac{N}{V} = \frac{g(mT)^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3} I(z), \quad I(z) = \int_0^\infty \frac{\sqrt{z}dz}{e^{(z-\mu/T)} - 1}$$

It increases with the temperature decrease and reaches zero at the temperature T_0 given by the equation

$$\frac{N}{V} = \frac{g(mT_0)^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3} I(0)$$

Since $I(0) = \left(\frac{\sqrt{\pi}}{2}\right)\zeta\left(\frac{3}{2}\right)$

where $\zeta(x)$ is the Riemann's ζ function

$$T_0 \approx \frac{3.31}{g^{\frac{2}{3}}} \frac{\hbar^2}{m}\left(\frac{N}{V}\right)^{\frac{2}{3}}$$

From above equations we obtain

$$(\beta T_0)^{\frac{3}{2}} = I(z)/I(0)$$

Chemical potential can be found by graphical solution above equation.

The above equation is based on replacement of the summation over discrete states by the integration. This is not true for bosons because they can *condense* in the ground state with $\varepsilon_k = 0$ We omit this term in our integration because $\sqrt{\varepsilon_k} = 0$ for

.

the ground state.

As a result, at $T < T_0$ the particles with $\varepsilon_k > 0$ are distributed according to the BE distribution with $\mu = 0$

$$dn_\varepsilon = \frac{gVm^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{\varepsilon}d\varepsilon}{e^{\beta(\varepsilon)} - 1}$$

The total number of such particles is

$$N_{\varepsilon>0} = \frac{gVm^{\frac{3}{2}}}{2^{\frac{1}{2}}\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{\varepsilon}d\varepsilon}{e^{\beta(\varepsilon)} - 1} = N\left(\frac{T}{T_0}\right)^{\frac{3}{2}}$$

and

$$N_{\varepsilon=0} = N[1 - \left(\frac{T}{T_0}\right)^{\frac{3}{2}}]$$

particles are in the lowest state with zero energy. The energy and other thermodynamic quantities can be obtained from general expression for Bose gas by putting $\mu = 0$. In this way we obtain

$$U = 0.770\, NT\left(\frac{T}{T_0}\right)^{\frac{3}{2}}$$

$$C_V = \frac{5U}{3T}$$

$$F = U - TS = -\left(\frac{2}{3}\right)U = \Omega\, since\, \mu = 0$$

$$P = -\left(\frac{\partial F}{\partial V}\right)_T = \frac{0.0851gm^{\frac{3}{2}}T^{\frac{5}{2}}}{\hbar^3}$$

Thus at $T \leq T_0$ ***the pressure is*** $\propto T^{5/2}$ and it is volume independent. The reason is that the particles in the condensate do not contribute to the pressure.

19.6 Self Learning Exercise- I

Short Answer Type Questions

Q.1 What is the mean occupation n_{level} of a bosonic level?

Q.2 Prove that pressure of a degenerate Bose gas is volume independent.

Q.3 Define Bose gas of elementary particle and derive ideal gas equation.

Q.4 Bosons, unlike fermions, are not subject to the ……

Q.5 State Pauli Exclusion Principle.

Q.6 Define Bose–Einstein condensate matter.

Long Answer Type Questions

Q.7 Discuss the temperature dependence of the energy, specific heat and entropy of an ideal Bose gas.

19.7 Black body distribution

The most important application of Bose statistics relates to electromagnetic radiation which is in thermal equilibrium is called Black body radiation. Take an empty box in contact with a reservoir of temperature *T*. The reservoir can interact with the box by emitting electromagnetic (EM) field waves into it. In quantum language we say that photons can travel into the box. ***The photons carry energy*** $\hbar\omega$, with $\omega = c|\boldsymbol{k}|$. Which **k** vectors are accessible is determined by the shape of the box. If we take a cube of size L^3, the **k** vectors are $\frac{2\pi}{L}(n_x, n_y, n_z)$ with N_i integer. From the quantum theory of the electromagnetic field, it follows that the photons are created and annihilated freely, so that there number cannot be controlled by a chemical potential. Creating a new photon in particular does not involve any cost except for its energy, so $\boxed{\mu = 0}$

Therefore, the number of modes available at frequency ω is given by

$$N(k)dk = 2.\frac{4\pi k^2 dk L^3}{(2\pi)^3} = \frac{V\omega^2 d\omega}{c^3\pi^2}$$

In this expression, ***the factor of 2 arises from the fact that there are two transverse modes*** (only transverse modes are allowed by Maxwell's equations), and we have divided the volume of the spherical shell with thickness *dk* in **k**-space

by the volume $\left(\frac{2\pi}{L}\right)^3$ of each **k**-point, and used $\omega = ck$. Now we use the fact that ***the photons are bosons (they are spin-1 particles***) and we have for the energy radiated at frequencies between ω and $\omega + d\omega$

$$dE_\omega = u(\omega)d\omega = n(\omega)\hbar\omega d\omega = \frac{V\hbar}{\pi^2 c^3}\frac{\omega^3 d\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

where the BE distribution is recognised, multiplied by the energy of the mode and the occupancy.

This formula for the spectral energy distribution of black body radiation is called Plank's formula. In terms of the wavelength $\lambda = 2\pi c/\omega$, it becomes

$$\boldsymbol{dE_\lambda = u(\lambda)d\lambda = \frac{16\pi^2 Vc\hbar}{\lambda^5}\frac{d\lambda}{e^{\frac{2\pi\hbar c}{T\lambda}} - 1}}$$

At low frequency ($\hbar\omega \ll T$)

$$\boldsymbol{dE_\omega = \frac{VT}{\pi^2 c^3}\omega^2 d\omega}$$

This is Rayleigh- Jeans formula. This formula does not contain the quantum constant $\hbar$, and can be derived by multiplying by T the number of modes, in this sense it corresponds to classical statistics. In classical statistics , energy T must correspond to each vibrational degree of freedom- The law of equipartition.

And at high frequency ($\hbar\omega \gg T$)

$$\boldsymbol{dE_\omega = \frac{V\hbar}{\pi^2 c^3} e^{-\frac{\hbar\omega}{k_B T}} \omega^3 d\omega}$$

This is Wien's formula.

The density of the spectral frequency distribution of the energy of black body radiation, $\frac{dE_\omega}{d\omega}$, has a maximum at a frequency $\omega_{\text{m given by}}$

$$\frac{\hbar\omega}{T} = 2.822$$

Thus when T rises, the position of the maximum of distribution is displaced towards higher frequencies in proportion to T.

Now let us calculate the thermodynamic quantities for the black body radiation.

For μ=0

$$F = \frac{TV}{\pi^2 c^3}\int_0^\infty \omega^2 \log\left(1 - e^{-\frac{\hbar\omega}{T}}\right) d\omega$$

Let $\frac{\hbar\omega}{T} = x$

$$F = \frac{-VT^4}{3\pi^2\hbar^3 c^3}\int_0^\infty \frac{x^3 dx}{e^x - 1}$$

Where $\int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$

$$F = \frac{-VT^4}{3\pi^2\hbar^3 c^3}\frac{\pi^4}{15} = -4\sigma\frac{VT^4}{3c}$$

Where σ=5.67 $\times 10^{-5}$ gm/sec^{3}deg^4 is Stefan Boltzmann constant.

The entropy is

$$S = -\frac{\partial F}{\partial T} = 16\sigma\frac{VT^3}{3c}$$

The total radiation energy

$$E = 4\sigma\frac{VT^4}{c} = -3F$$

This is Boltzmann's formula.

Specific heat of the radiation

$$C_v = \left(\frac{\partial E}{\partial T}\right)_v = \frac{16\sigma T^3 V}{c}$$

Pressure

$$P = -\frac{\partial F}{\partial V} = 4\sigma\frac{T^4}{3c}$$

and hence $\boxed{PV = \frac{E}{3}}$

19.8 Self Learning Exercise -II

Short Answer Type Questions

Q.1 Define Black body radiation.

Q.2 Apply the Bose- Einstein statistics to photons and obtain the Planck law of black body radiation.

Q.3 Write down Planks formula in terms of wavelength.

Q.4 State equipartition theorem.

Q.5 Draw Plank's distribution formula.

Q.6 Prove that the total radiation energy is proportional to the fourth power of temperature.

19.9 Summary

This unit started with the introduction of the Bose distribution followed by Bose gas of elementary particles and degenerate Bose gas. In this unit we also discussed Black body radiation and Plank's distribution formula.

19.10 Glossary

Degenerate: Describes an equilibrium assemblage whose variance is lower than expected from the number of phases and components because some other restriction is active in the phase rule. Examples include coincidences, singular points, collinear phases, and equilibria in which some or all phases are restricted to a bounding subsystem.

Blackbody: A blackbody is an object that absorbs all incident electromagnetic radiation and re-radiates it after reaching thermal equilibrium. The spectrum of light emitted by a blackbody is smooth and continuous, and depends on the blackbody's temperature. The peak of the spectrum is higher and at a shorter wavelength as the temperature increases.

***Bose-Einstein condensate*:** A Bose-Einstein condensate, or BEC, is a special phase of matter in which the quantum mechanical wavefunctions of a collection of particles line up and overlap in a manner that allows the particles to act as a single quantum object. The electrons in a superconductor form a BEC; superfluid helium is an example of a liquid BEC. BECs can also be created from dilute gases of ultra cold atoms and molecules.

***Elementary particles*:** Elementary particle is one of fundamental particles of which matter is composed, such as the electron, proton or neutron.

***Critical Point*:** The boundary between pressure or temperature conditions where a phase has an unstable region and pressure or temperature conditions where the phase is continuously stable. The critical point is the termination of a spinodal and

a solvus. The conditions of criticality reduce the variance by two; hence in a one-component system a critical point is invariant whereas in a binary system criticality is univariant and there is a family of critical points along a critical line.

***Fermion*:** A fermion is a particle with half-integer spin. The quarks and leptons of the Standard Model are fermions with a spin of 1/2. Composite particles can also be fermions. Baryons, such as protons and neutrons, and atoms of the alkali metals are all fermions. See: alkali metal, baryon, boson, lepton, spin.

***Boson*:** The collective name given to the particles that have integer (whole number) spin and carry forces between particles of matter.

***Pauli exclusion principle*: T**he Pauli exclusion principle is the principle that two particles of a specified type aren't able to be in the same

19.11 Answer to Self Learning Exercise

Answer to Self Learning Exercise I

Ans.1: In thermal equilibrium with a heat bath of temperature T and in contact with a particle reservoir with chemical potential μ the mean occupation is given by the Bose distribution

$$n_{level} = \frac{1}{exp\,\beta(E_{level} - \mu) - 1}$$

Ans.2: Section 19.5

$$P = -\left(\frac{\partial F}{\partial V}\right)_T = \frac{0.0851 g m^{\frac{3}{2}} T^{\frac{5}{2}}}{\hbar^3}$$

Ans.3:

$$\text{PV} = NT\left[1 - \frac{\pi^{\frac{3}{2}} N\hbar^3}{2gVT^{\frac{3}{2}} m^{\frac{3}{2}}}\right]$$

We see that the deviation of an ideal gas from classical properties, occurring when the temperature is lowered at constant density (degenerate).

Ans.4: Pauli Exclusion Principle

Ans.5: No two particles of half- integer spin (fermions) in an atom can have identical quantum numbers.

Ans.6: In 1924 Einstein pointed out that bosons could "condense" in unlimited numbers into a single ground state since they are governed by Bose-Einstein

statistics and not constrained by the Pauli exclusion principle. This state of matter was called a Bose-Einstein condensate.

Ans.7: Section 19.4

Answer to Self Learning Exercise-II

Ans.1: The most important application of Bose statistics relates to electromagnetic radiation which is in thermal equilibrium is called Black body radiation.

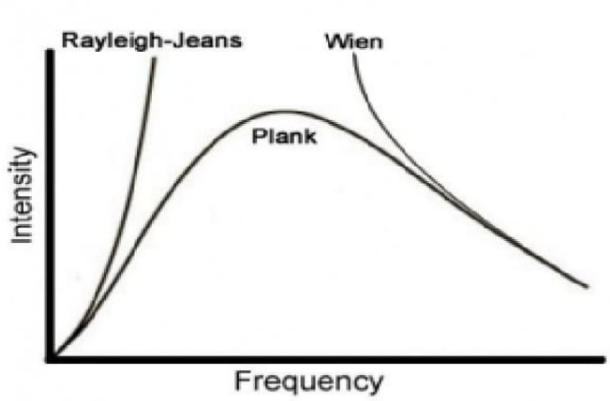
Ans.2: Section 19.7

Ans.3:

$$u(\lambda)d\lambda = \frac{16\pi^2 Vc\hbar}{\lambda^5} \frac{d\lambda}{e^{\frac{2\pi\hbar c}{T\lambda}} - 1}$$

Ans.4: In classical statistical mechanics, the equipartition theorem is a general formula that relates the temperature of a system with its average energies.

Ans.5:



Ans.6: $E = 4\sigma\frac{VT^4}{c} = -3F$

19.12 Exercise

Q.1 Derive the Plank's radiation formula assuming "The Bose-Einstein statistics for the photons".

Q.2 A collection of non-interacting bosons is kept at a temperature T. When the temperature is 0.4K, a fraction 26/27 of the total number of particles is in the ground state. If the temperature is increased to 0.9 K, what fraction of particles will be in the ground state?

Q.3 Consider a cubical box of sides L. what is the lowest energy of a system consisting of 10 free particles in this box if the particles obey Bose-Einstein statistics. (consider the spin degeneracy of the particles).

Q.4 Show that for an ideal Bose gas

$$\frac{1}{z}\left(\frac{\partial z}{\partial T}\right)_P = -\frac{5}{2T}\frac{g_{\frac{5}{2}}(z)}{g_{\left(\frac{3}{2}\right)}(z)}$$

Q.5 The velocity of sound in a fluid is given by the formula

$$w = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_s}$$

where ρ is the mass density of the fluid. Show that for an ideal Bose gas

$$w^2 = \frac{5kT}{3m}\frac{g_{\frac{5}{2}}(z)}{g_{\left(\frac{3}{2}\right)}(z)} = \frac{5}{9} < u^2 >$$

where $< u^2 >$ is the mean square speed of the particles in the gas.

Q.6 Show that the mean energy per photon in a blackbody radiation cavity is very nearly $2.7kT$.

References and Suggested Readings

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