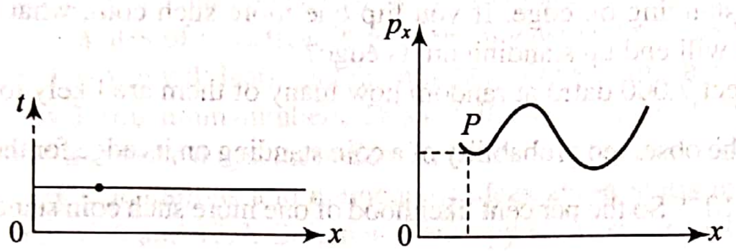
12.3 Phase Space and Quantum States

Let us consider the motion of a particle along a straight line (Fig. 12.1a). The mechanical state of the particle at any instant is given by its position x from a fixed point on the straight line and its velocity $v_x = \frac{dx}{dt}$ at that instant. However, (in view of uncertainty principle) it is more desirable to work with momentum $p_x(= mv_x)$ instead of velocity. As the particle moves along the straight line, the values of x and p_x change. So the state of the particle at any instant is completely specified classically at a particular instant if its position and momentum are known. It may be represented by any point P on a two-dimensional hypothetical space, whose coordinate axes are x and p_x (Fig. 12.1b). With the passage of time, the point P traces out a certain trajectory in the $x - p_x$ plane.



(a) (b)

Fig. 12.1 (a) Motion of a particle along a straight line and (b) Phase space for one-dimensional motion.

The state of the particle is referred to as the *phase*, the point P as the *phase point*, the trajectory as the *phase path* and the hypothetical two-dimensional plane as the *phase space*. These concepts are illustrated in the following example.

Example 12.2 Determine the phase path for a linear harmonic oscillator.

Solution: Suppose the mass and the force constant of the oscillator are m and k, respectively. From your school physics, you may recall that the total energy E of a linear harmonic oscillator is given by

$$E = \frac{1}{2}mv_x^2 + \frac{1}{2}kx^2$$

Since, $p_x = mv_x$, we can write $\frac{1}{2}mv_x^2 = \frac{p_x^2}{2m}$

so that we can write

$$E = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

or

$$\frac{p_x^2}{2mE} + \frac{x^2}{2(E/k)} = 1$$

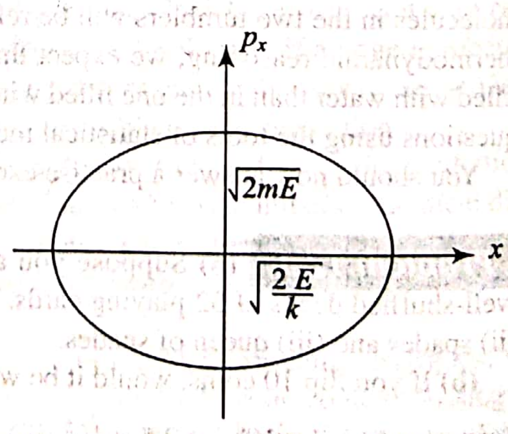


Fig.12.2 Phase path for a linear harmonic oscillator.

Since E is constant, $2mE$ and $2E/k$ are also constant. So this relation indicates that the phase point of the oscillator traces out an ellipse (Fig.12.2) in the x–p_x plane with semi-major and semi-minor axes equal to $\sqrt{2E/k}$ and $\sqrt{2mE}$ respectively.

Any point on this ellipse represents the phase at that time. As the oscillator moves to and fro along a straightline periodically, the same positions and momenta are repeated. So the phase point describes the ellipse of Fig. 12.2 over and over again.

In this example, the trajectory is a closed path. It may not always be so (Problem 12.2). But the curve will not intersect itself in any case.

Problem 12.2 A stone at rest falls freely. Determine its phase trajectory.

Ans: A parabola

You will note that the actual motion of a linear harmonic oscillator takes place along a straightline. An actual mechanical system is, in general, more complex than a particle moving along a straightline. A general treatment demands three position coordinates (x, y, z) and three components of momentum (p_x, p_y, p_z). In other words, we require six numerical quantities to specify the state of a system at a particular instant. That is, we need six-dimensional phase space. (Figure 12.1 only gives a symbolic representation of such a space.) It is referred to as μ–space. The state of translational motion of a molecule at any instant is completely specified by a representative point in this hypothetical space and the state of a system of particles corresponds to a certain distribution of points in phase space. For a system of N molecules, the instantaneous state is represented by a set of N points. As the position and momentum change with time, all these points may undergo extremely complicated motions in this space.

Note that the notion of phase space provides geometrical framework of some sort to statistical mechanics and helps to minimise abstraction. You will agree that it is not possible to draw such a space on a plane and for this reason, phase space should be considered a purely mathematical concept.

The uncertainty principle helps us to elaborate what we mean by a point in phase space. Suppose we divide the phase space into small six-dimensional cells of sides Δx, Δy, Δz, Δp_x, Δp_y, Δp_z. If we reduce the size of the cells, we approach more and more closely to the limit of a point in phase space. However, the volume of each of these cells is

$$H = \Delta x \Delta y \Delta z \Delta p_x \Delta p_y \Delta p_z$$

According to the uncertainty principle, the uncertainty in position and momentum coordinates in two-dimensional $x - p_x$ phase space is connected as

$$\Delta x \Delta p_x \geq \hbar \tag{12.1a}$$

where $\hbar = \dfrac{h}{2\pi}$; h is Planck's constant.

Identical relations hold for y and z-components:

$$\Delta y \Delta p_y \geq \hbar \tag{12.1b}$$

and

$$\Delta z \Delta p_z \geq \hbar \tag{12.1c}$$

On combining Eqs. (12.1 a–c), we can say that

$$H \geq \hbar^3 \tag{12.2}$$

We can now conclude that a point in phase space is a six-dimensional cell (or 'quantum box') whose volume is of the order of $\hbar^3$. A more detailed analysis shows that each cell in phase space has volume h^3, which is in conformity with the uncertainty principle argument since $h^3 > \hbar^3$. It means that a particle in phase space will be located somewhere in such a cell centred at some location (x, y, z, p_x, p_y, p_z) instead of being precisely at the point itself.

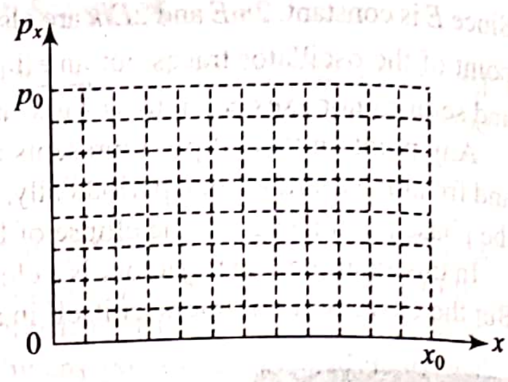


Fig. 12.3 The total number of states available to a particle confined between $0 \le x \le x_0$ and $0 \le p_x \le p_0$.

For simplicity, let us consider a particle moving along the x-direction. Let it be confined between $x = 0$ and $x = x_0$ and have its x – component of momentum between $p_x = 0$ and $p_x = p_0$ (Fig. 12.3). The number of states available to the particle in two-dimensional space is given by

$$n = \frac{\text{Total area}}{\Delta x \, \Delta p_x} = \frac{x_0 \, p_0}{h} \tag{12.3}$$

Similarly, we can say that the number of states available in six-dimensional phase space is given by

$$n = \frac{\text{Total six-dimensional volume}}{\Delta x \Delta y \Delta z \, \Delta p_x \, \Delta p_y \, \Delta p_z} = \frac{V_r \, V_p}{h^3} \tag{12.4}$$

where V_r and V_p denote the volumes in coordinate and momentum space, respectively. The number of states available in the six-dimensional volume element $d^3r \, d^3p$ is given by $\frac{d^3r \, d^3p}{h^3}$. Mathematically, we can write

$$\text{Number of states} = \frac{dx \, dy \, dz \, dp_x \, dp_y \, dp_z}{h^3} \tag{12.5}$$

From this we can say that the number of quantum states included in any interval of any of the coordinates is directly proportional to the length of the interval.

To give you an appreciation of the numbers, we give below a solved example. Go through it carefully.

Example 12.3 Calculate the number of quantum states available to the following:

(a) A particle is moving in one dimension. It is confined to 10^{-5}m of space and its momentum lies between -10^{-25} kg ms^{-1} and 10^{-25} kg ms^{-1}.

(b) A proton inside a nucleus (radius = 10^{-14}m) whose momentum cannot exceed 10^{-19} kg ms^{-1}.

Solution: (a) From Eq. (12.3), we recall that the number of quantum states available to a particle moving in one dimension is given by

$$n = \frac{x_0 \, p_0}{h} \tag{i}$$

Here $x_0 = 10^{-5}$ m, and $p_0 = 2 \times 10^{-25}$ kg ms^{-1}. Hence,

$$n = \frac{(10^{-5}\ \text{m}) \times (2 \times 10^{-25}\ \text{kg m s}^{-1})}{(6.626 \times 10^{-34}\ \text{Js})} = 3{,}000$$

(b) Since a proton inside a nucleus is free to move in 6 – *D* space, from Eq. (12.4), we can write

$$n = \frac{V_r V_p}{h^3} \tag{ii}$$

We know that $V_r = \frac{4\pi}{3} r_0^3$ with $r_0 = 10^{-14}$ m and $V_p = \frac{4\pi}{3} p_0^3$ with $p_0 = 10^{-19}$ kg m s^{-1}.

On substituting this data in Eq. (ii), we get

$$n = \frac{[(4\pi/3) \times 10^{-42}\ \text{m}^3] \times [(4\pi/3) \times 10^{-57}\ \text{kg}^3\,\text{m}^3\,\text{s}^{-3}]}{(6.626 \times 10^{-34}\ \text{Js})^3} = 600$$