Chapter 1

Classical and Quantum Mechanics: A Brief Review

Chapter Outline

In this overview we will study the Lagrangian and Hamiltonian formulations of the engineering mechanics starting from the principle of least action. It is emphasized that all the three formulations of classical mechanics are essentially the same, in that their domains of validity and predictions are identical. Nevertheless, the Hamiltonian formulation gives the ideal springboards to make the leap to quantum mechanics and complex mechanics. The central tool used in this book is the Hamilton mechanics, which is the only thing we need to know while we develop quantum mechanics, relativistic mechanics, and relativistic quantum mechanics. Before we solve quantum mechanical problems by Hamilton mechanics, several Key features of quantum mechanics will be reviewed in this chapter, such as the Schrodinger's equation, the Born's probability interpretation of wavefunction, the Heisenberg's uncertainty principle, tunneling phenomenon, and the energy quantization in one-dimensional box.

1.1 Principle of Least Action and Lagrange Mechanics

Let us take as our prototype of the Newtonian scheme a point particle of mass m moving along the x axis under a potential $V(x)$. According to Newton's second law, the particle's classical position $x_{\rm cl}(t)$ satisfies

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx} \tag{1.1.1}$$

If we are given the initial position $x(t_0) = x_0$ and the initial velocity $\dot{x}(t_0) = \dot{x}_0$, we can calculate the classical trajectory $x_{\rm cl}(t)$. The above scheme readily generalizes to more than one particle and more than one dimension. If we use n Cartesian coordinates $(x_1, x_2, \cdots, x_n)$ to specify the positions of the particles, the spatial configuration of the system may be visualized as a point in an n-dimensional configuration space. The motion of a representative point in this configuration space is given by

$$m_j\frac{d^2x_j}{dt^2} = -\frac{dV}{dx_j} \tag{1.1.2}$$

where m_j stands for the mass of the particle whose coordinate is x_j.

In the Lagrangian formalism, the problem of a single particle in a potential $V(x)$ is posed in a different way: given that the particle is at x_0 and x_f at times t_0 and t_f, respectively, what is it that distinguishes the actual trajectory $x_{\rm cl}(t)$ from all other trajectories or paths that connect these points ? (see Fig.1.1.1) The Lagrangian approach is thus global, in that it tries to determine at one stroke the entire $x_{\rm cl}(t)$, in contrast to the local approach of the Newtonian scheme, which concerns itself with what the particle is going to do in the next infinitesimal time interval.

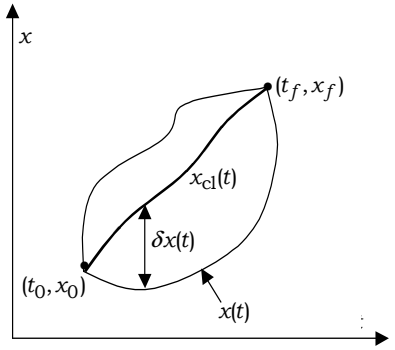

Fig. 1.1.1 The Lagrangian formalism asks what distinguishes the actual path $x_{\rm cl}(t)$ taken by the particle from all possible paths connecting the end points (t_0, x_0) and (t_f, x_f).

The answer to the question posed above comes in three parts:

(1) Define a function $L(t, x(t), \dot{x}(t))$, called the Lagrangian, given by

$$L = T - V \tag{1.1.3}$$

with T and V being the kinetic and potential energies of the particle.

(2) For each path $x(t)$ connecting (t_0, x_0) and (t_f, x_f), calculate the action $S[x(t)]$ defined by

$$S[x(t)] = \int_{t_0}^{t_f} L(t, x(t), \dot{x}(t))\, dt \tag{1.1.4}$$

We use square brackets to enclose the argument of S to remind us that the function S depends on an entire path or function $x(t)$, and not just the value of x at some time t. One calls S a functional to signify that it is a function of a function.

(3) The classical path $x_{\rm cl}(t)$ is the one on which S is an extremum, i.e., the variation of S, δS, with respect to arbitrary perturbation $\delta x(t)$ must be zero

$$\delta S[x(t)] = \delta\left(\int_{t_0}^{t_f} L(t, x(t), \dot{x}(t))\, dt\right) = 0 \tag{1.1.5}$$

The quantity S to be varied has the dimension of an action (energy•time); therefore, Eq. (1.1.5) is called principle of minimum action, and also called Hamilton principle which says that a system moves in such a way that the time integral over the Lagrangian takes an extreme value.

To derive the Lagrange equation of motion from the Hamilton principle (1.1.5), let's consider a system described by the generalized coordinates q_α, $\alpha = 1, 2, \cdots, n$, and the generalized velocities $\dot{q}_\alpha$. Starting from the integral

$$\delta S = \delta \int_{t_0}^{t_f} L(t, q_\alpha(t), \dot{q}_\alpha(t))\, dt = 0, \quad \alpha = 1,\ 2,\ \cdots,\ n\,, \tag{1.1.6}$$

we describe the variation of a path curve $q_\alpha(t)$ by

$$q_\alpha(t) \to q_\alpha(t) + \delta q_\alpha(t) \tag{1.1.7}$$

where the perturbation δq_α vanish at the endpoints, $\delta q_\alpha(t_0) = \delta q_\alpha(t_f) = 0$, since the endpoints are fixed. Since the fixed end time is not being varied, we have

$$\delta \int_{t_0}^{t_f} L\, dt = \int_{t_0}^{t_f} \delta L\, dt = \int_{t_0}^{t_f} \left(\sum_{\alpha=1}^{n} \frac{\partial L}{\partial q_\alpha} \delta q_\alpha + \sum_{\alpha=1}^{n} \frac{\partial L}{\partial \dot{q}_\alpha} \delta \dot{q}_\alpha \right) dt \tag{1.1.8}$$

The integration by part of the second summand yields

$$\int_{t_0}^{t_f} \frac{\partial L}{\partial \dot{q}_\alpha} \delta \dot{q}_\alpha\ dt = \int_{t_0}^{t_f} \frac{\partial L}{\partial \dot{q}_\alpha} \frac{d}{dt} \delta q_\alpha\ dt = \left[\frac{\partial L}{\partial \dot{q}_\alpha} \delta q_\alpha \right]_{t_0}^{t_f} - \int_{t_0}^{t_f} \left(\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\alpha} \right) \delta q_\alpha\ dt$$

Since δq_α vanishes at the endpoints (integration limits), we get for the variation of the integral

$$\delta S = \int_{t_0}^{t_f} \left(\sum_{\alpha=1}^{n} \left(\frac{\partial L}{\partial q_\alpha} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\alpha} \right) \delta q_\alpha \right) dt = 0$$

Because the δq_α's are arbitrary and independent of each other, the above integral vanishes only if the coefficient of any δq_α vanishes. This means that the Lagrange equations of motion hold:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\alpha} - \frac{\partial L}{\partial q_\alpha} = 0, \quad \alpha = 1,\ 2,\ \cdots,\ n \tag{1.1.9}$$

This is the celebrated Euler-Lagrange equation. If we feed into it

$$L = T - V = \frac{1}{2}\sum_{\alpha=1}^{n} m\dot{x}_\alpha^2 - V(x_1, x_2, \cdots, x_n)\,, \tag{1.1.10}$$

we get

$$\frac{\partial L}{\partial \dot{x}_\alpha} = \frac{\partial T}{\partial \dot{x}_\alpha} = m_\alpha \dot{x}_\alpha, \quad \frac{\partial L}{\partial x_\alpha} = -\frac{\partial V}{\partial x_\alpha},$$

so that the Euler-Lagrange equation becomes just

$$m_\alpha \frac{d^2 x_\alpha}{dt^2} = -\frac{dV}{dx_\alpha}, \quad \alpha = 1,\ 2,\ \cdots,\ n\,, \tag{1.1.11}$$

which is identical to Eq.(1.1.2). Thus the least action principle indeed reproduces Newtonian mechanics if we choose $L = T - V$.

Example 1.1.1

This is an example with a constraint. A chain of constant density σ (mass per unit length: $\sigma = dm\,/\,ds$) and length l hangs in the gravitational field between two points $P_1(x_1, y_1)$ and $P_2(x_2, y_2)$. We look for the form of the curve, assuming that the potential energy of the chain takes a minimum.

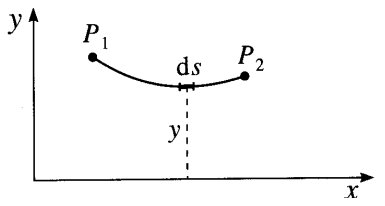

Fig.1.1.1. A Chain hangs in the gravitational field.

Answer：

The potential energy of a chain element is $dV = g\sigma y ds$. The action $S[y(x)]$ to be minimized is the total potential energy

$$S[y(x)] = V = g\sigma \int_{x_1}^{x_2} y ds = g\sigma \int_{x_1}^{x_2} y\sqrt{dx^2 + dy^2}$$
$$= g\sigma \int_{x_1}^{x_2} y\sqrt{1 + (dy\,/\,dx)^2}\,dx = g\sigma \int_{x_1}^{x_2} y\sqrt{1 + y'^2}\,dx, \quad y' = \frac{dy}{dx}$$

The constraint of given length l is represented by

$$0 = \int_{x_1}^{x_2} ds - l = \int_{x_1}^{x_2} \sqrt{1 + y'^2}\,dx - l$$

Introducing the Lagrange multiplier λ in the action S to include the constraint, we have

$$S = g\sigma \int_{x_1}^{x_2} y\sqrt{1 + y'^2}\,dx - \lambda\left(\int_{x_1}^{x_2} \sqrt{1 + y'^2}\,dx - l \right)$$

Then the variation of S becomes

$$\delta S = \delta \int_{t_0}^{t_f} L\ dt = 0, \quad L = (y - \mu)\sqrt{1 + y'^2}, \quad \mu = \lambda\,/(g\sigma)$$

From the Euler-Lagrange equation

$$\frac{d}{dx}\frac{\partial L}{\partial y'} - \frac{\partial L}{\partial y} = 0\,,$$

it follows that

$$(y-\mu)y'' - y'^2 - 1 = 0$$

With the help of the identity

$$y'' = \frac{dy'}{dx} = \frac{dy'}{dy}\frac{dy}{dx} = y'\frac{dy'}{dy},$$

we can rewrite the Euler-Lagrange equation as

$$\frac{dy}{y-\mu} = \frac{y'dy'}{1+y'^2}$$

Integration yields

$$\ln(y-\mu) + \ln A = (1/2)\ln(1+y'^2) \quad \Rightarrow \quad A(y-\mu) = \sqrt{1+y'^2}$$

From this, we get

$$\int \frac{dy}{\sqrt{A^2(y-\mu)^2 - 1}} = \int dx$$

To integrate the left side, we substitute the change of variable

$$\cosh z = A(y-\mu), \quad dy = (1/A)\sinh z dz\,,$$

then the integration is reduced to

$$z = A(x+B) \quad \Rightarrow \quad y = (1/A)\cosh(A(x+B)) + \mu$$

Thus, the solution is the catenary. The lowest point (x_0, y_0) of the chain is given by $(x_0, y_0) = (-B, \mu + 1/A)$ with the two constants A and B determined by the given length l of the chain and by the suspension points P_1 and P_2.

□

The term $\partial L/\partial q_\alpha = -\partial V/\partial q_\alpha = Q$ in Eq.(1.1.9) is known as generalized force and the term $\partial L/\partial \dot{q}_\alpha = p_\alpha$ is regarded as the generalized momentum. We therefore can interpret Eq.(1.1.9) as

$$\frac{d}{dt}(\text{generalized momentum}) = \text{generalized force} \quad \Rightarrow \quad \frac{dp_\alpha}{dt} = Q \tag{1.1.12}$$

In terms of this interpretation, we thus can conceive of Lagrange equation as the generalized Newton's second law. The generalized coordinate q_α is called an ignorable or cyclic coordinate, if $\partial L/\partial q_\alpha = 0$. The Lagrange equation (1.1.9) for this case reduces to

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\alpha} = \frac{d}{dt}p_\alpha = 0 \quad \Rightarrow \quad p_\alpha = \text{constant} \tag{1.1.13}$$

The generalized momentum p_α related to the cyclic coordinate is thus constant in time; in other words, the generalized momentum related to a cyclic coordinate is conserved.

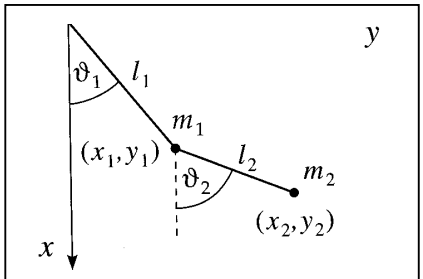

Fig.1.1.2 Coordinates of the double pendulum.

Example 1.1.2

The double pendulum as shown in Fig.1.1.2 consists of two end masses m_1 and m_2 connected by two rods with negligible mass. The problem is to derive the equations of motion for the two point masses and to find their linearized motions.

Answer:

The appropriate generalized coordinates are the two angles θ_1 and θ_2 that are related to the Cartesian coordinates by

$$x_1 = l_1\cos\theta_1, \quad y_1 = l_1\sin\theta_1, \quad x_2 = l_1\cos\theta_1 + l_2\cos\theta_2, \quad y_2 = l_1\sin\theta_1 + l_2\sin\theta_2$$

The velocity components in Cartesian coordinates are obtained by differentiation

$$\dot{x}_1 = -l_1\dot{\theta}_1\sin\theta_1, \quad \dot{y}_1 = l_1\dot{\theta}_1\cos\theta_1, \quad \dot{x}_2 = -l_1\dot{\theta}_1\sin\theta_1 - l_2\dot{\theta}_2\sin\theta_2, \quad \dot{y}_2 = l_1\dot{\theta}_1\cos\theta_1 + l_2\dot{\theta}_2\cos\theta_2$$

from which the kinetic energy of the system is found to be

$$T = \frac{m_1}{2}(\dot{x}_1^2 + \dot{y}_1^2) + \frac{m_2}{2}(\dot{x}_2^2 + \dot{y}_2^2) = \frac{m_1}{2}m_1 l_1^2\dot{\theta}_1^2 + \frac{m_2}{2}\Big[l_1^2\dot{\theta}_1^2 + l_2^2\dot{\theta}_2^2 + 2l_1l_2\dot{\theta}_1\dot{\theta}_2\cos(\theta_1-\theta_2)\Big]$$

To get the potential energy, we adopt a plane as the reference height at the distance $l_1 + l_2$ below the suspension point:

$$V = m_1 g(l_1 + l_2 - l_1\cos\theta_1) + m_2 g\big[l_1 + l_2 - (l_1\cos\theta_1 + l_2\cos\theta_2)\big]$$

The Lagrangian then becomes

$$\begin{aligned} L = T - V = {} & \frac{m_1}{2}m_1 l_1^2\dot{\theta}_1^2 + \frac{m_2}{2}\Big[l_1^2\dot{\theta}_1^2 + l_2^2\dot{\theta}_2^2 + 2l_1l_2\dot{\theta}_1\dot{\theta}_2\cos(\theta_1-\theta_2)\Big] \\ & - m_1 g(l_1 + l_2 - l_1\cos\theta_1) - m_2 g\big[l_1 + l_2 - (l_1\cos\theta_1 + l_2\cos\theta_2)\big] \end{aligned}, \tag{1.1.14}$$

from which the various differentiations can be evaluated as

$$\frac{\partial L}{\partial\theta_1} = -m_2 l_1 l_2\dot{\theta}_1\dot{\theta}_2\sin(\theta_1-\theta_2) - m_1 g l_1\sin\theta_1 - m_2 g l_1\sin\theta_1$$

$$\frac{\partial L}{\partial\dot{\theta}_1} = m_1 l_1^2\dot{\theta}_1 + m_2 l_1^2\dot{\theta}_1 + m_2 l_1 l_2\dot{\theta}_2\cos(\theta_1-\theta_2)$$

$$\frac{\partial L}{\partial\theta_2} = m_2 l_1 l_2\dot{\theta}_1\dot{\theta}_2\sin(\theta_1-\theta_2) - m_2 g l_2\sin\theta_2, \quad \frac{\partial L}{\partial\dot{\theta}_2} = m_2 l_2^2\dot{\theta}_2 + m_2 l_1 l_2\dot{\theta}_1\cos(\theta_1-\theta_2)$$

Substituting the above differentiations into the Lagrange equation for θ_1 and θ_2

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}_1}\right) - \frac{\partial L}{\partial\theta_1} = 0, \quad \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}_2}\right) - \frac{\partial L}{\partial\theta_2} = 0\,,$$

we obtain

$$\begin{aligned} (m_1+m_2)l_1^2\ddot{\theta}_1 + m_2 l_1 l_2\ddot{\theta}_2\cos(\theta_1-\theta_2) + m_2 l_1 l_2\dot{\theta}_2^2\sin(\theta_1-\theta_2) &= -(m_1+m_2)g l_1\sin\theta_1 \\ m_2 l_2^2\ddot{\theta}_2 + m_2 l_1 l_2\ddot{\theta}_1\cos(\theta_1-\theta_2) - m_2 l_1 l_2\dot{\theta}_1^2\sin(\theta_1-\theta_2) &= -m_2 g l_2\sin\theta_2 \end{aligned}$$

For the case of $m_1 = m_2 = m$ and $l_1 = l_2 = l$, the above equations reduce to

$$\begin{aligned} 2l\ddot{\theta}_1 + l\ddot{\theta}_2\cos(\theta_1-\theta_2) + l\dot{\theta}_2^2\sin(\theta_1-\theta_2) &= -2g\sin\theta_1 \\ l\ddot{\theta}_1\cos(\theta_1-\theta_2) + l\ddot{\theta}_2 - l\dot{\theta}_1^2\sin(\theta_1-\theta_2) &= -g\sin\theta_2 \end{aligned} \tag{1.1.15}$$

If moreover the oscillations are small, then $\sin\theta \approx \theta$, $\cos\theta \approx 1$, and terms proportional to $\dot{\theta}^2$ are negligible, which leads to

$$2l\ddot{\theta}_1 + l\ddot{\theta}_2 = -2g\theta_1, \quad l\ddot{\theta}_1 + l\ddot{\theta}_2 = -g\theta_2 \tag{1.1.16}$$

With the ansatz, $\theta_1(t) = A_1 e^{i\omega t}$, $\theta_2(t) = A_2 e^{i\omega t}$, we then obtain

$$2(g - l\omega^2)A_1 - l\omega^2 A_2 = 0, \quad -l\omega^2 A_1 + (g - l\omega^2)A_2 = 0\,. \tag{1.1.17}$$

To ensure that A_1 and A_2 do not vanish simultaneously, the determinant of the coefficients must vanish:

$$\begin{vmatrix} 2(g-l\omega^2) & -l\omega^2 \\ -l\omega^2 & g - l\omega^2 \end{vmatrix} = 0\,,$$

which has two solutions

$$\omega_1^2 = (2+\sqrt{2})g/l, \quad \omega_2^2 = (2-\sqrt{2})g/l\,. \tag{1.1.18}$$

By inserting Eq.(1.1.18) into Eq.(1.1.17), we obtain the out-of-phase solution $A_2 = -\sqrt{2}A_1$ if $\omega = \omega_1$,

and the in-phase solution $A_2 = \sqrt{2}A_1$, if $\omega = \omega_2$.

1.2 Hamilton Mechanics

In the Lagrangian formalism, the independent variables are the coordinates q_α and the velocities $\dot{q}_\alpha$. The momenta are derived quantities defined by

$$p_\alpha = \frac{\partial L}{\partial \dot{q}_\alpha} \tag{1.2.1}$$

In the Hamiltonian formalism one exchange the roles of $\dot{q}$ and p; one replaces the Lagrangian $L(t, q, \dot{q})$ by a Hamiltonian $H(t, q, p)$ which generates the equation of motion, and $\dot{q}$ becomes a derived quantity,

$$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} \tag{1.2.2}$$

thereby completing the role reversal of the $\dot{q}_\alpha$'s and p_α's. The Hamiltonian H can be constructed from the Lagrangian L via the relation

$$H(t, q_\alpha, p_\alpha) = \sum_\alpha p_\alpha \dot{q}_\alpha - L(t, q_\alpha, p_\alpha) \tag{1.2.3}$$

We look for those equations of motion, which are equivalent to the Lagrange equations based on the Lagrangian L. To this end, we form the total differential:

$$dH = \sum_\alpha p_\alpha d\dot{q}_\alpha + \sum_\alpha \dot{q}_\alpha dp_\alpha - dL\,, \tag{1.2.4}$$

The total differential dL of the Lagrangian reads

$$dL(t, q_\alpha, \dot{q}_\alpha) = \sum \frac{\partial L}{\partial q_\alpha} dq_\alpha + \sum \frac{\partial L}{\partial \dot{q}_\alpha} d\dot{q}_\alpha + \frac{\partial L}{\partial t} dt = \sum \dot{p}_\alpha dq_\alpha + \sum p_\alpha d\dot{q}_\alpha + \frac{\partial L}{\partial t} dt\,, \tag{1.2.5}$$

where we have utilized the definition of the generalized momentum $p_\alpha = \partial L / \partial \dot{q}_\alpha$ as given in Eq.(1.2.1) and the Lagrange equation in the form

$$\dot{p}_\alpha = \frac{d}{dt} p_\alpha = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\alpha} = \frac{\partial L}{\partial q_\alpha} \tag{1.2.6}$$

Inserting Eq.(1.2.5) into Eq.(1.2.4) yields

$$dH = \sum_\alpha \dot{q}_\alpha dp_\alpha - \sum_\alpha \dot{p}_\alpha dq_\alpha - \frac{\partial L}{\partial t} dt \tag{1.2.7}$$

On the other hand, since $H = H(t, q_\alpha, p_\alpha)$, we have an alternative differential form for H:

$$dH = \sum \frac{\partial H}{\partial q_\alpha} dq_\alpha + \sum \frac{\partial H}{\partial p_\alpha} dp_\alpha + \frac{\partial H}{\partial t} dt \tag{1.2.8}$$

Equating Eq.(1.2.7) and Eq.(1.2.8), we obtain the Hamilton equations

$$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha}, \quad \dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha}, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \tag{1.2.9}$$

The Hamiltonian H plays the central role, similar to the Lagrangian L in Lagrange's formulation of mechanics. This Hamiltonian H is constructed according to Eq.(1.2.3); but with the prescription that all the velocities $\dot{q}_\alpha$'s are expressed by the generalized momenta p_α and the generalized coordinates q_α. This can be done by solving $\dot{q}_\alpha$ from Eq.(1.2.1)

$$p_\alpha = \frac{\partial L(t, q_\alpha, \dot{q}_\alpha)}{\partial \dot{q}_\alpha} \quad \Rightarrow \quad \dot{q}_\alpha = \dot{q}_\alpha(q_\alpha, p_\alpha) \tag{1.2.10}$$

The $\dot{q}_\alpha$ obtained this way are inserted into the definition of H in Eq.(1.2.3), so that the Hamiltonian H finally depends only on q_α, p_α, and t; hence, $H = H(t, q_\alpha, p_\alpha)$. From this, the Hamilton equations are established and solved.

The Lagrange equations provide a set of n differential equations of second order in the time for the position coordinates. The Hamiltonian formalism yields $2n$ coupled differential equations of first order for the momentum and position coordinates. In any case, there are $2n$ integration constants when solving the system of equations. Table 1.2.1 provides a comparison of the Lagrangian and Hamiltonian formalisms.

Table 1.2.1 Comparison of the Lagrangian and Hamiltonian Formalism

Lagrangian Formalism	**Hamiltonian Formalism**
1. The state of a system with n degrees of freedom is described by n coordinates $(q_1,\cdots,q_n)$ and n velocities $(\dot{q}_1,\cdots,\dot{q}_n)$, or in a more compact notation by $(q,\dot{q})$.	1. The state of a system with n degrees of freedom is described by n coordinates and n momenta $(q_1,\cdots,q_n,p_1,\cdots,p_n)$ or more succinctly, by (q,p).
2. The state of the system may be represented by a point moving with a definite velocity in an n-dimensional configuration space.	2. The state of the system may be represented by a point in a $2n-$dimensional phase space, with coordinates $(q_1,\cdots,q_n,p_1,\cdots,p_n)$.
3. The n coordinates evolve according to n second-order equations.	3. The $2n$ coordinates and momenta obey $2n$ first-order equations.
4. For a given L, several trajectories may pass through a given point in configuration space depending on $\dot{q}$.	4. For a given H only one trajectory passes through a given point in phase space.

In the above discussion we have derived the Hamilton equations from the Lagrange equations. Here we wish to show that Hamilton equations can be deduced directly from the Hamilton principle. We first express the Lagrangian L in terms of the Hamiltonian H from Eq.(1.2.3) as

$$L(t,q_\alpha,p_\alpha)=\sum_\alpha p_\alpha\dot{q}_\alpha - H(t,q_\alpha,p_\alpha) \tag{1.2.11}$$

Then Eq.(1.1.6) becomes

$$\delta S=\int_{t_0}^{t_f}\delta L dt=\int_{t_0}^{t_f}\sum_\alpha\left[\delta p_\alpha\dot{q}_\alpha+p_\alpha\delta\dot{q}_\alpha-\frac{\partial H}{\partial p_\alpha}\delta p_\alpha-\frac{\partial H}{\partial q_\alpha}\delta q_\alpha\right]dt \tag{1.2.12}$$

The second term on the right-hand side can be transformed by integration by parts,

$$\int_{t_0}^{t_f}p_\alpha\delta\dot{q}_\alpha\ dt=\int_{t_0}^{t_f}p_\alpha\frac{d}{dt}\delta q_\alpha\ dt=p_\alpha\delta q_\alpha|_{t_0}^{t_f}-\int_{t_0}^{t_f}\dot{p}_\alpha\delta q_\alpha\ dt\,,$$

where the first term vanishes since the variation at the endpoints vanish： $\delta q_\alpha(t_0)=\delta q_\alpha(t_f)=0$. Hence, Eq.(1.2.12) becomes

$$0=\int_{t_0}^{t_f}\delta L dt=\int_{t_0}^{t_f}\sum_\alpha\left[\left(\dot{q}_\alpha-\frac{\partial H}{\partial p_\alpha}\right)\delta p_\alpha+\left(-\dot{p}_\alpha-\frac{\partial H}{\partial q_\alpha}\right)\delta q_\alpha\right]dt \tag{1.2.13}$$

Since the variations δp_α and δq_α are independent of each other along a path in phase space, the condition $\delta S=0$ requires

$$\begin{aligned}\dot{q}_\alpha&=\frac{\partial H}{\partial p_\alpha},\quad q_\alpha(0)=q_{\alpha_0}\\ \dot{p}_\alpha&=-\frac{\partial H}{\partial q_\alpha},\quad p_\alpha(0)=p_{\alpha_0}\end{aligned} \tag{1.2.14}$$

Again we arrive at the same Hamilton equations as already derived in Eq.(1.2.9). Note that we have altogether $2n$ first-order equations for a system with n degrees of freedom. Given the initial-value data, $(q_\alpha(0),p_\alpha(0))$, $\alpha=1,2,\cdots,n$, we can integrate the equations to get $(q_\alpha(t),p_\alpha(t))$. It is seen from Eq.(1.2.14) that for a coordinate that does not enter into the Hamiltonian, the corresponding change of the momentum with time vanishes:

$$\partial H/\partial q_i=0\quad\Rightarrow\quad p_i=\text{constant}\,. \tag{1.2.15}$$

We then call q_i the ignorable or cyclic coordinate.

Now, just as L may be interpreted as $T-V$ if the force is conservative, so there exists a

simple interpretation for H in this case. Consider the sum $\sum p_\alpha \dot{q}_\alpha$. Let us use Cartesian coordinates, in terms of which

$$T = \sum_{\alpha=1}^{n} \frac{1}{2} m_\alpha \dot{x}_\alpha^2 \quad \Rightarrow \quad p_\alpha = \frac{\partial L}{\partial \dot{x}_\alpha} = \frac{\partial T}{\partial \dot{x}_\alpha} = m_\alpha \dot{x}_\alpha, \quad \sum_{\alpha=1}^{n} p_\alpha \dot{x}_\alpha = \sum_{\alpha=1}^{n} m_\alpha \dot{x}_\alpha^2 = 2T$$

so that the Hamiltonian

$$H = \sum_{\alpha=1}^{n} p_\alpha \dot{x}_\alpha - L = 2T - (T - V) = T + V \tag{1.2.16}$$

can be identified as the total energy of the system. Note that although we used Cartesian coordinates along the way, the resulting equation (1.2.16) is a relation among scalars and thus coordinate independent. If the considered system is conservative, it is natural that the total energy $H = T + V$ is a constant. Since

$$\frac{dH}{dt} = \sum \frac{\partial H}{\partial q_i} \dot{q}_i + \sum \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial t}$$

and with the Hamilton equation (1.2.14) this leads to

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} . \tag{1.2.17}$$

Therefore, for a conservative system the Hamiltonian H shall not be explicitly time dependent, since then $dH / dt = \partial H / \partial t = 0$ and thus, $H =$ constant .

One can easily derive Newton's equations from Hamilton's equations and thus show the equivalence of both formulations. It is sufficient to consider a single particle in a conservative force field and to use the Cartesian coordinates as generalized coordinates. Then

$$p_\alpha = m\dot{x}_\alpha, \quad H = \frac{m}{2} \sum_\alpha \dot{x}_\alpha^2 + V(x_\alpha) \quad \Rightarrow \quad H = \frac{1}{2m} \sum_\alpha p_\alpha^2 + V(q_\alpha) \tag{1.2.18}$$

This leads to the Hamilton equations ($q_\alpha = x_\alpha$):

$$\dot{q}_\alpha = \frac{\partial H}{\partial p_\alpha} = \frac{p_\alpha}{m}, \quad \dot{p}_\alpha = -\frac{\partial H}{\partial q_\alpha} = -\frac{\partial V}{\partial q_\alpha}, \quad \alpha = 1,2,3 \tag{1.2.19}$$

or in vector notation

$$m \frac{d^2 \boldsymbol{q}}{dt^2} = \frac{d}{dt}\left(m \frac{d\boldsymbol{q}}{dt} \right) = \frac{d}{dt} \boldsymbol{p} = -\nabla V \tag{1.2.20}$$

These are Newton's equations of motion.

Example 1.2.1

Derive the equations of motion of the pendulum within the frames of Newton's, Lagrange's, and Hamilton's theory.

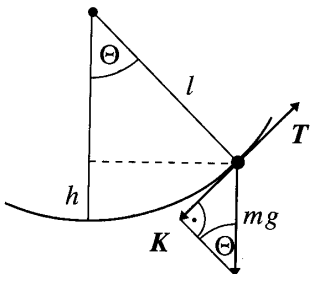

Fig.1.2.1 Force balance in pendulum motion.

Answer:

• Newtonian theory:

The arc length of the displacement is denoted by s , and the tangent unit vector by $\boldsymbol{T}$. Then Newton's second law gives (refer to Fig.1.2.1)

$$m\ddot{s}\boldsymbol{T} = \boldsymbol{K} = -(mg \sin\theta)\boldsymbol{T} .$$

With $s = l\theta$, we have $\ddot{s} = l\ddot{\theta}$. We therefore get the equation of motion

$$\ddot{\theta} + (g / l) \sin\theta = 0$$

For small displacements with $\sin\theta \approx \theta$, the above equation becomes $\ddot{\theta} + (g / l)\theta = 0$, which has the general solution

$$\theta(t) = A \cos\sqrt{g / l}\, t + B \sin\sqrt{g / l}\, t ,$$

where the constants A and B are to be determined from the initial conditions.

- Lagrangian Theory:

$$T = (1/2)mv^2 = (1/2)m(l\dot{\theta})^2, \quad V = mgh = mgl(1-\cos\theta)$$

Hence, the Lagrangian for this conservative system reads

$$L = T - V = (1/2)ml^2\dot{\theta}^2 - mgl(1-\cos\theta)$$

Now we use the Lagrange equation

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

With $\partial L/\partial\theta = -mgl\sin\theta, \quad \partial L/\partial\dot{\theta} = ml^2\dot{\theta}$, we have $\ddot{\theta} + (g/l)\sin\theta = 0$.

- Hamiltonian Theory:

Using the generalized momentum $p_\theta = \partial L/\partial\dot{\theta} = ml^2\dot{\theta}$, the kinetic energy can be written as

$$T = \frac{1}{2}ml^2\dot{\theta}^2 = \frac{1}{2}\frac{p_\theta^2}{ml^2}$$

Since the total energy of the system is constant, the Hamiltonian reads

$$H = T + V = \frac{1}{2}\frac{p_\theta^2}{ml^2} + mgl(1-\cos\theta)$$

The Hamilton equations yield

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ml^2}, \quad \frac{dp_\theta}{dt} = -\frac{\partial H}{\partial\theta} = -mgl\sin\theta$$

Combining the above two equations leads to

$$\frac{d}{dt}p_\theta = \frac{d}{dt}\left(ml^2\dot{\theta}\right) = -mgl\sin\theta\,,$$

which finally reduces to $\ddot{\theta} + (g/l)\sin\theta = 0$.

1.3 Canonical Transformations and Hamilton-Jacobi Theory

Given a Hamiltonian $H = H(q_i, p_i, t)$, the motion of the system is found by integrating the Hamilton equations:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{1.3.1}$$

For the case of a cyclic coordinate, we have

$$\frac{\partial H}{\partial q_i} = 0 \quad \Rightarrow \quad \dot{p}_i = 0$$

Hence, the corresponding momentum is constant: $p_i = \beta_i = \text{constant}$. Whether or not H contains cyclic coordinates depends in general on the coordinates adopted for describing a problem. For example, if a circular motion in a central field is described in Cartesian coordinates (x, y), there is no cyclic coordinate; while if we use polar coordinates (r, θ), the angular coordinate θ is cyclic.

A mechanic problem would therefore be greatly simplified if one could find a coordinate transformation from the set (p_i, q_i) to a new set of coordinates (P_i, Q_i) with

$$Q_i = Q_i(p_i, q_i, t), \quad P_i = P_i(p_i, q_i, t) \tag{1.3.2}$$

where all coordinates Q_i for the problem were cyclic with respect to the new Hamiltonian $\mathscr{H}$, i.e., $\partial\mathscr{H}/\partial Q_i = 0$. Then all the momenta in the new coordinates are constant, $P_i = \beta_i = \text{constant}$. For such a case, the new Hamiltonian $\mathscr{H}$ is only a function of the constant momenta P_i; hence, $\mathscr{H} = \mathscr{H}(P_i)$. Then.

$$\dot{Q}_i = \frac{\partial\mathscr{H}(P_i)}{\partial P_i} = \omega_i = \text{constant}, \quad \dot{P}_i = -\frac{\partial\mathscr{H}(P_i)}{\partial Q_i} = 0 \tag{1.3.3}$$

Then integration with respect to time leads to

$$Q_i = \omega_i t + \omega_0, \quad P_i = \beta_i = \text{constant} \tag{1.3.4}$$

Inserting Q_i and P_i back to Eq.(1.3.2) and solving for p_i and q_i, we can find $q_i(t)$ and $p_i(t)$, and the mechanic problem is then solved. That is to say, we can solve a mechanic problem merely by coordinate transformation without solving directly the differential equations in Eq.(1.3.1). The remaining problem is how to find the special transformation possessing the property (1.3.3).

In this section we look for a canonical transformation to coordinates $P_i = p_{i0}$ and $Q_i = q_{i0}$ which all are constant and are given by the initial conditions. When we have found such coordinates, the transformation equations are solutions of the system in the normal position coordinates:

$$q_i = q_i(Q_j, P_j, t) = q_i(q_{j0}, p_{j0}, t), \quad p_i = p_i(Q_j, P_j, t) = p_i(q_{j0}, p_{j0}, t) \tag{1.3.5}$$

The new coordinates (P_i, Q_i) obey the Hamilton equations with the new Hamiltonian $\mathcal{H}(Q_i, P_i, t)$. Since the time derivatives vanish by definition, we have

$$\dot{Q}_i = 0 = \frac{\partial \mathcal{H}}{\partial P_i}, \quad \dot{P}_i = 0 = -\frac{\partial \mathcal{H}}{\partial Q_i} \tag{1.3.6}$$

These conditions would certainly be fulfilled by the function

$$\mathcal{H} = 0 \tag{1.3.7}$$

In order to find such a special transformation, we need a generating function S. We adopt the solution $S(q_i, P_i, t)$ suggested by Jacobi, which meets the following transformation:

$$p_i = \frac{\partial S}{\partial q_i}(q_j, P_j, t), \quad Q_i = \frac{\partial S}{\partial P_i}(q_j, P_j, t) \tag{1.3.8a}$$

$$\mathcal{H}(P_i, Q_i, t) = H(p_i, q_i, t) + \frac{\partial S}{\partial t}(q_i, P_i, t) \tag{1.3.8b}$$

The requirement that the new Hamiltonian shall vanish, $\mathcal{H} = 0$, leads to:

$$\frac{\partial S}{\partial t} + H\left(q_1, \cdots, q_n, p_1 = \frac{\partial S}{\partial q_1}, \cdots, p_n = \frac{\partial S}{\partial q_n}, t\right) = \mathcal{H} = 0 \tag{1.3.9}$$

Writing down this equation with the arguments, we obtain

$$\frac{\partial S(q_i, P_i = \beta_i, t)}{\partial t} + H\left(q_1, \cdots, q_n, \frac{\partial S}{\partial q_1}, \cdots, \frac{\partial S}{\partial q_n}, t\right) = 0 \tag{1.3.10}$$

This is the Hamilton-Jacobi differential equation, which is a nonlinear partial differential equation of first order with $n+1$ variables q_1, q_2, $\cdots$, q_n, and t. To get the action function S, we have to integrate the differential equation $n+1$ times (each derivative of $\partial S / \partial q_i$ and $\partial S / \partial t$ requires one integration), and we thus obtain $n+1$ integration constants. But since S appears in the differential equation only as a derivative, S is determined only up to a constant. This means that one of the $n+1$ integration constants must be a constant additive to S. It is, however, not essential for the transformation. We thus obtain a solution in the form of

$$S = S(q_1, \cdots, q_n; \beta_1, \cdots, \beta_n, t)\,, \tag{1.3.11}$$

where the β_i's are integration constants. The combination of Eq.(1.3.6) with Eq.(1.3.8a) leads to the requirement:

$$P_i = \beta_i, \quad Q_i = \frac{\partial S}{\partial P_i} = \frac{\partial S(q_1, \cdots, q_n; \beta_1, \cdots, \beta_n; t)}{\partial \beta_i} = \alpha_i, \quad i = 1, 2, \cdots n \tag{1.3.12}$$

Once S is solved from Eq.(1.3.10), the original coordinates $(q_i(t), p_i(t))$ can be determined as follows. From the second equation of Eq.(1.3.12), the position coordinates q_i can be solved in terms of α_i, β_i, and t:

$$q_i = q_i(\alpha_j, \beta_j, t) \tag{1.3.13}$$

Inserting this result into Eq.(1.3.8a) yields

$$p_i = \frac{\partial S(q_j, P_j, t)}{\partial q_j} = p_i(q_j, \beta_j, t) = p_i(\alpha_j, \beta_j, t) \tag{1.3.14}$$

Now $q_i = q_i(\alpha_j, \beta_j, t)$ and $p_i = p_i(\alpha_j, \beta_j, t)$ are determined as functions of time and of the integration constants α_j and β_j, which are evaluated by initial conditions. Therefore we have seen that the mechanical problem is automatically solved, once the solution of Hamilton-Jacobi equation (1.3.10) is found.

If H is not an explicit function of time, the considered system is conservative, and in the meantime H represents the total energy E of the system. In this case, Eq.(1.3.10) reduces to

$$-\partial S / \partial t = H = E\,, \tag{1.3.15}$$

from which S can be represented as

$$S(q_i, \beta_i, t) = S_0(q_i, \beta_i) - Et \tag{1.3.16}$$

To explain the meaning of S, we form the total derivative of S with respect to time:

$$\frac{dS}{dt} = \sum \frac{\partial S}{\partial q_i}\dot{q}_i + \sum \frac{\partial S}{\partial P_i}\dot{P}_i + \frac{\partial S}{\partial t}\,, \tag{1.3.17}$$

By inserting the fact

$$p_i = \frac{\partial S}{\partial q_i}, \quad \dot{P}_i = 0, \quad \frac{\partial S}{\partial t} = -H\,,$$

we obtain

$$\frac{dS}{dt} = \sum p_i \dot{q}_i - H(q_i, p_i, t) = L(q_i, p_i, t) \tag{1.3.18}$$

This means that S is given by the time integral over the Lagrangian:

$$S = \int L(q_i, p_i, t)\ dt + \text{constant} \tag{1.3.19}$$

Since this integral physically represents an action （energy • time） as defined in Eq.（1.1.4）, the solution S of the Hamilton-Jacobi equation in Eq.(1.3.10) is indeed an action function. However, Eq.(1.3.19) can not be used for a practical calculation of S, since as long as the problem is not yet solved, one does not know L as a function of time.

Example 1.3.1

A harmonic oscillator has the following Hamiltonian

$$H(q, p) = (1/2m)p^2 + (k/2)q^2\,. \tag{1.3.20}$$

By applying this $H(q, p)$ in Eq.(1.3.10), find the solution $S(q, \beta, t)$ and use it to determine $q(t)$.

Answer：

The Hamilton-Jacobi equation has the form

$$\frac{\partial S}{\partial t} + H(q, p, t)\big|_{p=\partial S/\partial q} = 0 \quad \Rightarrow \quad \frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{k}{2}q^2 = 0 \tag{1.3.21}$$

For solving the problem, we make a separation ansatz into a space and a time variable:

$$S = S_1(t) + S_2(q)$$

Substituting $\partial S / \partial q = dS_2(q)/dq$ and $\partial S / \partial t = dS_1(t)/dt$ into Eq.(1.3.21) leads to

$$-\dot{S}_1(t) = \frac{1}{2m}\left(\frac{dS_2(q)}{dq}\right)^2 + \frac{k}{2}q^2 = \beta\,.$$

The left side depends only on the time t, the right side only on the coordinate q; therefore, both

sides can only be equal if they are equal to a common constant β. For the time-dependent part, we have

$$\dot{S}_1(t) = -\beta \quad \Rightarrow \quad S_1(t) = -\beta t$$

For the space-dependent part, we have

$$\frac{1}{2m}\left(\frac{dS_2(q)}{dq}\right)^2 + \frac{k}{2}q^2 = \beta \quad \Rightarrow \quad \frac{dS_2}{dq} = \sqrt{2m\beta - mkq^2}$$

As sum of the two parts, we then obtain for S

$$S(q,\beta,t) = \sqrt{mk}\int \sqrt{2\beta\,/\,k - q^2}\; dq - \beta t \tag{1.3.22}$$

Employing this $S(q,\beta,t)$ in Eq.(1.3.12), we have the relation

$$\alpha = Q = \frac{\partial S}{\partial \beta} = \frac{\sqrt{mk}}{k}\int \left(2\beta\,/\,k - q^2\right)^{-1/2} dq - t$$

Evaluation of the integral results in

$$Q + t = \sqrt{m\,/\,k}\,\arcsin\left(\sqrt{k\,/\,(2\beta)}q\right)$$

With the usual abbreviation $\omega^2 = k\,/\,m$, we obtain the solution for $q(t)$:

$$q(t) = \sqrt{2\beta\,/\,k}\,\sin\omega(t+\alpha)\,. \tag{1.3.23}$$

This solution is in the same form obtained from solving the Newton equation with β related to the total energy E and α related to the initial time t_0.

1.4 Separable Solution of Hamilton-Jacobi PDE

The separation of the Hamilton-Jacobi equation represents a general (often the only feasible) way of solving it. If the Hamiltonian does not explicitly depend on the time, i.e., the considered system is conservative, then

$$\frac{\partial S}{\partial t} + H\left(q_1,\cdots,q_n,\frac{\partial S}{\partial q_1},\cdots,\frac{\partial S}{\partial q_n}\right) = 0 \tag{1.4.1}$$

and the time can be separated off immediately from S. We set for S a solution of the form

$$S(q_i,P_i,t) = S_0(q_i,P_i) - Et\,, \tag{1.4.2}$$

where the constant E represents the total energy of the system, as can be seen by inserting Eq.(1.4.2) into Eq.(1.4.1)

$$H\left(q_1,\cdots,q_n,\frac{\partial S_0}{\partial q_1},\cdots,\frac{\partial S_0}{\partial q_n}\right) = E = \text{constant}\,. \tag{1.4.3}$$

To achieve a separation of the position variables, we make the ansatz

$$S_0(q_1,\cdots,q_n,P_1,\cdots,P_n) = S_1(q_1,P_1) + \cdots + S_n(q_n,P_n)\,. \tag{1.4.4}$$

This means that the Hamilton action function splits into a sum of partial functions S_i, each depending only on one pair of variables (q_i,P_i). The Hamilton-Jacobi equation then becomes

$$H\left(q_1,\cdots,q_n,\frac{dS_1}{dq_1},\cdots,\frac{dS_n}{dq_n}\right) = E\,. \tag{1.4.5}$$

To ensure that this differential equation also separates into n differential equations, with each equation for one partial function $S_i(q_i,P_i)$, H must has the form

$$H(q_1,\cdots,q_n,p_1,\cdots,p_n) = H_1(q_1,p_1) + \cdots + H_n(q_n,p_n) \tag{1.4.6}$$

A Hamiltonian of this form describes a system of independent degrees of freedom. With Eq.(1.4.6), Eq.(1.4.5) reads

$$H_1\left(q_1, \frac{dS_1}{dq_1}\right) + \cdots + H_n\left(q_n, \frac{dS_n}{dq_n}\right) = E \tag{1.4.7}$$

This equation can be satisfied by setting each term H_i separately equal to a constant β_i:

$$H_1\left(q_1, \frac{dS_1}{dq_1}\right) = \beta_1, \quad H_2\left(q_2, \frac{dS_2}{dq_2}\right) = \beta_2, \quad \cdots, \quad H_n\left(q_n, \frac{dS_n}{dq_n}\right) = \beta_n \tag{1.4.8}$$

where

$$\beta_1 + \beta_2 + \cdots + \beta_n = E \tag{1.4.9}$$

Since the kinetic energy term of the Hamiltonian involves the momentum $p_i = dS_i / dq_i$ quadratically, the differential equations in Eq. (1.6.8) are of first order and second degree. As solutions, we then obtain the n action functions:

$$S_i = S_i(q_i, \beta_i) \tag{1.4.10}$$

According to Eq. (1.4.17a), S_i immediately leads to the conjugate momentum

$$p_i = \frac{dS_i(q_i, \beta_i)}{dq_i} \tag{1.4.11}$$

Hence for separable systems, the coordinate pair (q_i, p_i) is not coupled to any other coordinate pair (q_k, p_k), $k \neq i$, so that the motion in these coordinates can be considered fully independent of the other ones.

Example 1.4.1 Solving Kepler problem by the Hamilton-Jacobi method

Use the Hamilton-Jacobi method for solving the Kepler problem in a central force field of the form $V(r) = -K / r$.

Answer:

We adopt plane polar coordinates (r, θ) as generalized coordinates. The Hamiltonian has been determined in Example 1.3.1 with $V(r) = -k / r$ as

$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) - \frac{K}{r} \tag{1.4.12}$$

Since H is cyclic in θ, $p_\theta = \text{constant} = l$. The conjugate momenta can be expressed by the Hamilton action function S:

$$p_i = \frac{\partial S}{\partial q_i} \quad \Rightarrow \quad p_r = \frac{\partial S}{\partial r}, \quad p_\theta = \frac{\partial S}{\partial \theta} = \text{constant} = \beta_2$$

Thus we obtain the Hamilton-Jacobi differential equation:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \theta}\right)^2\right] - \frac{K}{r} = 0 \tag{1.4.13}$$

By adopting the separation of variable for S:

$$S = S_1(r) + S_2(\theta) + S_3(t), \tag{1.4.14}$$

Eq.(1.4.13) reduces to

$$\frac{1}{2m}\left[\left(\frac{dS_1}{dr}\right)^2 + \frac{1}{r^2}\left(\frac{dS_2}{d\theta}\right)^2\right] - \frac{K}{r} = -\frac{dS_3}{dt} = E \tag{1.4.15}$$

This equation can be satisfied only if both sides are constant. The constant is the total energy of the system, because

$$-\frac{\partial S}{\partial t} = H = E \quad \Rightarrow \quad -\frac{dS_3}{dt} = \text{constant} = \beta_3 = E \tag{1.4.16}$$

We remember that

$$P_i = \beta_i, \quad Q_i = \frac{\partial S}{\partial P_i} = \frac{\partial S}{\partial \beta_i} = \alpha_i$$

where α_i and β_i are constants to be determined from initial conditions. The other equation from Eq.(.4.15) is

$$\left(\frac{dS_2(\theta)}{d\theta}\right)^2 = r^2\left[2m\beta_3 + \frac{2mK}{r} - \left(\frac{dS_1(r)}{dr}\right)^2\right] \tag{1.4.17}$$

Both sides of above equation must be constant, and let it be denoted by β_2^2. Then we have

$$\frac{dS_2(\theta)}{d\theta} = \beta_2 = \text{constant}, \quad \frac{dS_1(r)}{dr} = \sqrt{2m\beta_3 + \frac{2mK}{r} - \frac{\beta_2^2}{r^2}} \tag{1.4.18a}$$

The Hamilton action function can now be written down as follows:

$$S = \int \sqrt{2m\beta_3 + 2mK\,/\,r - \beta_2^2\,/\,r^2}\;\; dr + \beta_2\theta - \beta_3 t \tag{1.4.18b}$$

We now define β_2 and β_3 as new momenta P_θ and P_r. The quantities Q_i conjugate to the P_i are also constant:

$$Q_r = \frac{\partial S}{\partial P_r} = \frac{\partial S}{\partial \beta_3} = \frac{\partial}{\partial \beta_3}\int \sqrt{2m\beta_3 + 2mK\,/\,r - \beta_2^2\,/\,r^2}\;\; dr - t = \alpha_3 \tag{1.4.19a}$$

$$Q_\theta = \frac{\partial S}{\partial P_\theta} = \frac{\partial S}{\partial \beta_2} = \frac{\partial}{\partial \beta_2}\int \sqrt{2m\beta_3 + 2mK\,/\,r - \beta_2^2\,/\,r^2}\;\; dr + \theta = \alpha_2 \tag{1.4.19b}$$

With the substitution $u = 1\,/\,r$, Eq.(1.4.19b) can be rewritten as

$$-\int \frac{du}{\sqrt{2mE\,/\,l^2 + (2mK\,/\,l^2)u - u^2}} = \theta - \alpha_2$$

The integration gives

$$r = \frac{l^2\,/(mK)}{1 + e\cos(\theta - \alpha_2 + \pi\,/\,2)}, \quad e = \sqrt{1 + \frac{2El^2}{mK^2}} \tag{1.4.20}$$

This is the solution of the Kepler problem. The types of trajectories follow from the eccentricity of the conic curves determined by the total energy E:
(1) $E = 0$: the orbit is a parabola with $e = 1$.
(2) $E < 0$: the orbit is an ellipse with $e < 1$.
(3) $E > 0$: the orbit is a hyperbola with $e > 1$

1.5 Schrodinger Equation and Born Interpretation

The central role of the quantum mechanics is played by the Schrödinger equation

$$i\hbar\frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)\,. \tag{1.5.1}$$

which is known as the time-dependent Schrödinger equation. The solutions $\Psi(x,t)$ of Eq.(1.5.1) are the time-dependent wave functions. An important goal in wave mechanics is solving Eq.(1.5.1) for $\Psi(x,t)$ using various expressions for $V(x)$ that relate to specific physical systems.

The relation of wave function $\Psi(x,t)$ with the motion of the associated particle was proposed by Max Born in 1926:
(A) The probability that a particle will be found in the infinitesimal interval dx about the point x, denoted by $f_x(x)dx$, is

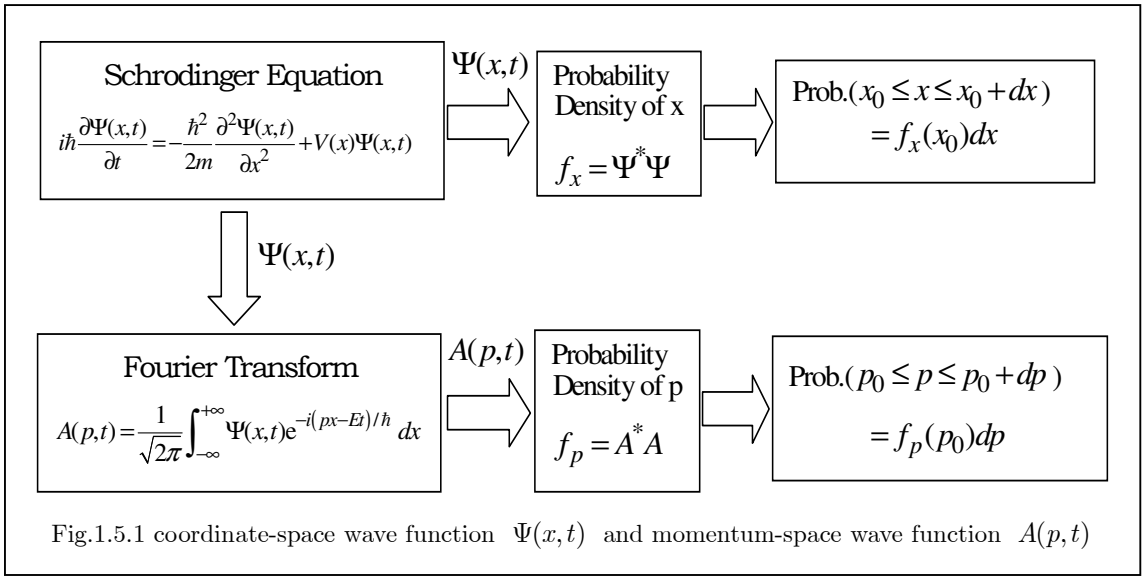

Fig.1.5.1 coordinate-space wave function $\Psi(x,t)$ and momentum-space wave function $A(p,t)$

$$f_x(x)dx=\Psi^*(x,t)\Psi(x,t)dx=\left|\Psi(x,t)\right|^2dx \tag{1.5.2}$$

(B) The probability that the momentum of a particle will be found in the infinitesimal interval dp about the point p, denoted by $f_p(p)dp$, is

$$f_p(p)dp=A^*(p,t)A(p,t)dx=\left|A(p,t)\right|^2dp \tag{1.5.3}$$

Note that Ψ is itself not a measurable quantity; however, $|\Psi|^2$ is measurable and is just the probability per unit length, called probability density function $f_x(x)$. Thus the wave function does not indicate the actual location at which the particle will be found, but rather provides the probability for finding the particle in any given interval. According to the Born's statistical interpretation, the wave function completely describes the physical system it represents. There is no information about the system that is not contained in $\Psi(x,t)$. Hence the state of the system is completely determined by its wave function. For this reason the wave function is also called the state function, or simply called "state".

Since the wave function $\Psi(x,t)$ completely describes the physical system that it represents, it Fourier transform $A(p,t)$ also possesses that property. Either function may serve as a complete description of the state of the system (see Fig.0.5.1)

Because its relation to probability, $\Psi(x,t)$ must satisfy

(1) both $\Psi(x,t)$ and $d\Psi(x,t)/dx$ are single valued.
(2) both $\Psi(x,t)$ and $d\Psi(x,t)/dx$ are continuous.
(3) both $\Psi(x,t)$ and $d\Psi(x,t)/dx$ are finite.

Fig.1.5.2 illustrates the meaning of these properties by plotting functions, which are not finite, not single valued, or not continuous, at point x_0. These conditions are required in order to have a unique probability density for every point in space and at all times. In order that $d\Psi(x,t)/dx$ be finite, it is necessary that $\Psi(x,t)$ be continuous. The necessity for $d\Psi(x,t)/dx$ to be continuous can be demonstrated by considering the time-independent Schrödinger equation:

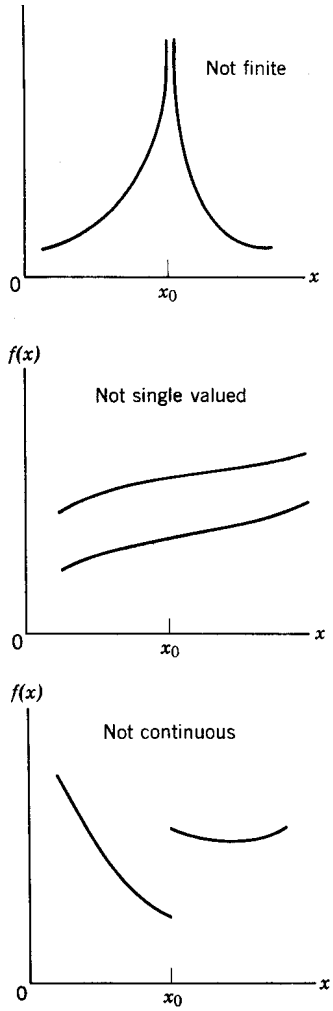

Fig.1.5.2. Functions which are not finite, not single valued, or not continuous at a point x_0.

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\psi(x)$$

(refer to the next section for detailed derivation). For finite $V(x)$, E, and $\Psi(x,t)$, we see that $d^2\Psi(x,t)/dx^2$ must be finite. This, in turn, demands that we require $d\Psi(x,t)/dx$ to be continuous because any function that has a discontinuity in the first derivative will have an infinite second derivative at the same point.

The importance of these requirements on the properties of acceptable solutions to the time-dependent Schrodinger equation cannot be overemphasized. Differential equations have a wide variety of possible solutions. It is only when we select from all the possible solutions those that conform to these requirements that we obtain energy quantization, or other equally significant properties of the Schrodinger theory that will be treated in the following sections.

Also since a particle must be somewhere along the x axis, the sum of the probabilities over all values of x must be 1:

$$\int_{-\infty}^{+\infty} \left|\Psi(x,t)\right|^2 dx = 1 \tag{1.5.4}$$

A function obeying this condition is said to be normalized. Normalization is simply a statement that the particle exists at all time. The probability of finding the particle in any finite interval $a \le x \le b$ is

$$P = \int_a^b \left|\Psi(x,t)\right|^2 dx \tag{1.5.5}$$

This probability is just the area included under the curve of probability density between the points $x = a$ and $x = b$. If a function $\Phi(x,t)$ is not normalized, but satisfies the relation

$$\int_{-\infty}^{+\infty} \Phi^*(x,t)\Phi(x,t)dx = N$$

then the function $\Psi(x,t)$ defined by $\Psi(x,t) = \Phi(x,t)/\sqrt{N}$ is normalized. In order for $\Psi(x,t)$ to be normalizable, the wave function must be quadratically integrable. Therefore, $\Psi(x,t)$ must go to zero faster than $1/\sqrt{N}$ as x approaches $(\pm)$ infinity. Likewise, the derivative $\partial\Psi/\partial x$ must also go to zero as x approaches infinity.

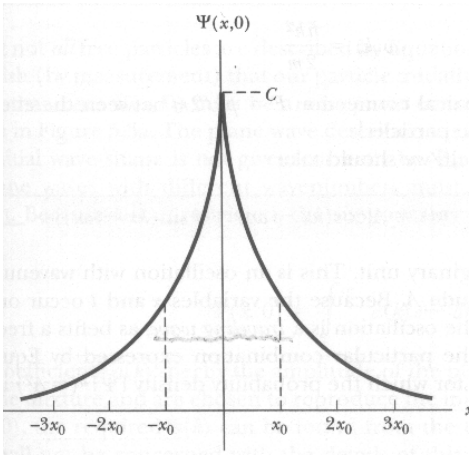

Fig.1.5.3. The wave function considered in example 1.5.1.

Example 1.5.1

The initial wave function of a particle is given as $\Psi(x,0) = C\exp(-|x|/x_0)$, where C and x_0 are constants. (a) Sketch this function, and find C in terms of x_0 such that $\Psi(x,0)$ is normalized. (b) Calculate the probability that the particle will be found in the interval $-x_0 \le x \le x_0$.

Answer:

(a) The given function is symmetric, decaying exponentially from the origin as shown in Fig.0.5.3. The decay length x_0 represents the distance over which the wave amplitude is diminished by the factor e^{-1} from its maximum value $\Psi(0,0) = C$. The normaliz- ation requirement is

$$1 = \int_{-\infty}^{+\infty} \left|\Psi(x,0)\right|^2 dx = C^2\int_{-\infty}^{+\infty} e^{-2|x|/x_0}dx = 2C^2\int_0^{\infty} e^{-2|x|/x_0}dx = 2C^2\left(x_0/2\right) = C^2x_0$$

Thus, we must take $C = 1/\sqrt{x_0}$ for normalization.

(b) The probability is the area under the curve of $\left|\Psi(x,0)\right|^2$ from $-x_0$ to $+x_0$, and is obtained by integrating the probability density over the specified interval:

$$P = \int_{-x_0}^{x_0} \left|\Psi(x,0)\right|^2 dx = 2\int_0^{x_0} \left|\Psi(x,0)\right|^2 dx = 2C^2\int_0^{x_0} e^{-2x/x_0}dx = 2C^2(x_0/2)(1-e^{-2})$$

Substituting $C = 1/\sqrt{x_0}$ into above expression gives the probability $P = 1 - e^{-2} = 0.8647$, or about 86.5%, independent of x_0.

1.6 Expectation Operations

In the domain of quantum mechanics, position, momentum, and many other physical quantities of a particle are uncertain due to its wave motion. What are certain and what we can evaluate deterministically are the mean values or expectation values of these physical quantities. Hence, learning to find the expectation value of a quantum variable is most important in the study of quantum mechanics. In this section we will investigate some operational rules of expectation. These expectation operations will then be used in the subsequent sections to describe the average motion of a particle.

1.6.1 Expectation of Coordinates

A particle described by the wave function Ψ may occupy various places x with probability given by the probability density $|\Psi(x)|^2$. Prediction made from Ψ can be tested by making repeated measurements of the particle's position. Table 1.6.1 shows results that might be obtained in a hypothetical experiment. The table consists of 18 entries, each one representing the actual position of the particle recorded in that particular measurement. We see that the entry 5.4 occurs most often (in 3 of the 18 trials); it represents the most probable position based on the data available. The probability associated with this position is 3/18=0.167. The information in Table 0.6.1 can be used to find the average position of the particle:

Table 1.6.1 Hypothetical Data Set for Position of a Particle in Repeated Trials

Trial	Position	Trial	Position	Trial	Position
1	$x_1 = 2.5$	7	$x_7 = 8.0$	13	$x_{13} = 4.2$
2	$x_2 = 3.7$	8	$x_8 = 6.4$	14	$x_{14} = 8.8$
3	$x_3 = 1.4$	9	$x_9 = 4.1$	15	$x_{15} = 6.2$
4	$x_4 = 7.9$	10	$x_{10} = 5.4$	16	$x_{16} = 7.1$
5	$x_5 = 6.2$	11	$x_{11} = 7.0$	17	$x_{17} = 5.4$
6	$x_6 = 5.4$	12	$x_{12} = 3.3$	18	$x_{18} = 5.3$

$$\overline{x} = (2.5 + 3.7 + 1.4 + \cdots + 5.4 + 5.3)/18 = 5.46$$

This same number can be found in a different way. First, order the table entries by value, starting with the smallest: 1.4, 2.5, 3.3, …, 5.4, 6.2, …, 8.0, 8.8. Now take each value, multiply by its frequency of occurrence, and sum the results:

$$\overline{x} = 1.4\left(\frac{1}{18}\right) + 2.5\left(\frac{1}{18}\right) + \cdots + 5.4\left(\frac{3}{18}\right) + 6.2\left(\frac{2}{18}\right) + \cdots + 8.8\left(\frac{1}{18}\right) = 5.46$$

The two procedures are equivalent, but the latter involves a sum over ordered pairs ($1.x$, P_x): (1.1.4, 1/18), (1.2.5, 1/18), …, (1.5.4, 3/18), …, (1.8.8, 1/18), rather than individual table entries. This latter expression allows us to write a general prescription to calculate the average particle position from any data set:

$$\overline{x} = \sum xP_x \tag{1.6.1}$$

The sum now includes all values of x, each weighted by its frequency or probability of occurrence P_x. If the possible values of x are distributed continuously over the entire range of real numbers, the sum and the probability must be replaced by

$$\sum \rightarrow \int , \quad P_x \rightarrow P(x)dx = \left|\Psi(x)\right|^2 dx$$

and Eq.(1.6.1) becomes

$$\langle x\rangle = \int_{-\infty}^{+\infty} xP(x)dx = \int_{-\infty}^{+\infty} x\left|\Psi(x,t)\right|^2 dx \tag{1.6.2}$$

$\langle x\rangle$ is the average value of x, called expectation value. More generally, the expectation value $\langle f(x)\rangle$ of any function $f(x)$ of the variable x is given by

$$\langle f(x)\rangle = \int_{-\infty}^{+\infty} f(x)\left|\Psi(x,t)\right|^2 dx = \int_{-\infty}^{+\infty} \Psi^*(x,t)f(x)\Psi(x,t)dx \tag{1.6.3}$$

Since $\Psi(x,t)$ depends on the time t, the expectation values $\langle x\rangle$ and $\langle f(x)\rangle$ are functions of time t.

Example 1.6.1
Consider $f(x) = (x - \langle x\rangle)^2$, find $\langle f(x)\rangle$. We call $\langle f(x)\rangle$ the variance of x, and $\langle f(x)\rangle^{1/2}$ the standard deviation of x.

Answer:

$$\begin{aligned}\langle f(x)\rangle &= \left\langle (x-\langle x\rangle)^2\right\rangle = \int_{-\infty}^{+\infty} (x-\langle x\rangle)^2\left|\Psi(x)\right|^2 dx \\ &= \int_{-\infty}^{+\infty} x^2\left|\Psi(x)\right|^2 dx - 2\langle x\rangle\int_{-\infty}^{+\infty} x\left|\Psi(x)\right|^2 dx + \langle x\rangle^2\int_{-\infty}^{+\infty}\left|\Psi(x)\right|^2 dx \\ &= \left\langle x^2\right\rangle - 2\langle x\rangle^2 + \langle x\rangle^2 = \left\langle x^2\right\rangle - \langle x\rangle^2\end{aligned}$$

The standard deviation $\langle f(x)\rangle^{1/2}$, denoted by Δx, is defined by

$$\Delta x = \sqrt{\left\langle (x-\langle x\rangle)^2\right\rangle} = \sqrt{\left\langle x^2\right\rangle - \langle x\rangle^2} \tag{1.6.4}$$

In section 1.6.4, we will see that the standard deviations Δx and Δp satisfy the uncertainty principle: $\Delta x\Delta p \geq \hbar/2$.

1.6.2 Expectation of Momentum

The expectation value $\langle p\rangle$ of the momentum p may be obtained using the momentum-space wave function $A(p,t)$ in the same way that $\langle x\rangle$ was obtained from $\Psi(x,t)$ as shown in Eq.(1.6.2):

$$\langle p\rangle = \int_{-\infty}^{+\infty} p\left|A(p,t)\right|^2 dp = \int_{-\infty}^{+\infty} pA^*(p,t)A(p,t)dp \tag{1.6.5}$$

The expectation value $\langle f(p)\rangle$ of any function $f(p)$ of p is given by an expression analogous to Eq.(1.6.5):

$$\langle f(p)\rangle = \int_{-\infty}^{+\infty} f(p)\left|A(p,t)\right|^2 dp \tag{1.6.6}$$

From Eq.(1.6.5) and Eq.(1.6.6) we see that in order to evaluate $\langle p\rangle$ or $\langle f(p)\rangle$ the Fourier transform $A(p,t)$ of $\Psi(x,t)$ must be found beforehand. A question now arise naturally: can we evaluate $\langle p\rangle$ or $\langle f(p)\rangle$ directly from $\Psi(x,t)$ without resorting to $A(p,t)$? The answer is confirmative, since both $\Psi(x,t)$ and $A(p,t)$ contain the same information about the system, making it possible to find $\langle p\rangle$ using the coordinate-space wave function $\Psi(x,t)$ in place of $A(p,t)$? From Eq.(1.6.2), we have

$$A(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\Psi(x,t)\mathrm{e}^{-i(px-Et)/\hbar}\ dx, \quad A^*(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\Psi^*(x,t)\mathrm{e}^{i(px-Et)/\hbar}\ dx$$

Substituting $A^*(p,t)$ into the integral on the right-hand side of Eq.(1.6.5) yields

$$\begin{aligned}\langle p\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\Psi^*(x,t)pA(p,t)e^{i(px-Et)/\hbar}dxdp \\ &= \int_{-\infty}^{+\infty}\Psi^*(x,t)\left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}pA(p,t)e^{i(px-Et)/\hbar}dp\right]dx\end{aligned} \tag{1.6.7}$$

where the integration in the bracket can be evaluated by applying the definition of $\Psi(x,t)$:

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}A(p)\mathrm{e}^{i(px-Et)/\hbar}\ dp \\ \Rightarrow \frac{\partial\Psi(x,t)}{\partial x} &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\frac{i}{\hbar}\,pA(p)\mathrm{e}^{i(px-Et)/\hbar}\ dp\end{aligned} \tag{1.6.8}$$

Substitution of this observation into Eq.(1.6.7) gives the final result

$$\langle p\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t)dx \tag{1.6.9}$$

Therefore, the expectation of momentum can be obtained by an integration in coordinate space.

The expectation of p^2 is given by Eq.(1.6.6) with $f(p)=p^2$. The expression analogous to Eq.(1.6.7) is

$$\left\langle p^2\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}p^2A(p,t)e^{i(px-Et)/\hbar}dp\right]dx$$

Similar to Eq.(1.6.8), the integration in square bracket equals

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\left(\frac{i}{\hbar}\right)^2 p^2A(p)\mathrm{e}^{i(px-Et)/\hbar}\ dp$$

therefore,

$$\left\langle p^2\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2\Psi(x,t)dx\,. \tag{1.6.10}$$

In the same manner, the expectation value of p^n is given by

$$\left\langle p^n\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\Psi(x,t)dx \tag{1.6.11}$$

By comparing with

$$\left\langle x^n\right\rangle = \int_{-\infty}^{+\infty}x^n\left|\Psi(x,t)\right|^2dx = \int_{-\infty}^{+\infty}\Psi^*(x,t)x^n\Psi(x,t)dx \tag{1.6.12}$$

we see that it is possible to treat the computation of $\left\langle p^n\right\rangle$ as that of $\left\langle x^n\right\rangle$ by defining the operator

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}\,. \tag{1.6.13}$$

In terms of $\hat{p}$, Eq.(1.6.11) can be rewritten in the form of Eq.(1.6.12):

$$\left\langle p^n\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{p}^n\Psi(x,t)dx\,.$$

Thus if we replace p by $\hat{p}$, all the computation of expectation regarding to p can be done in the same way as in the computation of $\langle x\rangle$, so that

$$\left\langle f(p)\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)f(\hat{p})\Psi(x,t)dx\,. \tag{1.6.14}$$

We may combine Eq.(1.6.3) and Eq.(1.6.14) to find the expectation value of a function $f(x,p)$ of the position and momentum

$$\left\langle f(x,p)\right\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)f(x,\hat{p})\Psi(x,t)dx = \int_{-\infty}^{+\infty}\Psi^*(x,t)f\left(x,\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t)dx\,. \tag{1.6.15}$$

1.6.3 Observables and Operators

An observable is any particle property that can be measured. The position and momentum of a particle are observables, as are its kinetic and potential energy. Quantum mechanics associates an operator with each of these observables. Using this operator, one can calculate the average value of the corresponding observable. An operator here refers to an operation to be performed on whatever function follows the operator. The quantity operated on is called the operand.

Table 0.6.2 Observables and Associated Operators

Observable	**Symbol**	**Operator**
Position	$\hat{x}$	x
Momentum	$\hat{p}$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
Potential Energy	$\widehat{V}$	$V(x)$
Kinetic Energy	$\widehat{K}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Hamiltonian	$\widehat{H}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$
Total Energy	$\widehat{E}$	$i\hbar\frac{\partial}{\partial t}$

For example, in Eq.(1.6.13) we have associated an operator $\hat{p}=(\hbar/i)(\partial/\partial x)$ with the momentum p via the operation

$$\hat{p}\Psi(x,t)=\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial x} \tag{1.6.16}$$

The wave function $\Psi(x,t)$, which is operated by $\hat{p}$, is called the operand of $\hat{p}$. We can see that $\hat{p}$ is indeed a differential operator. Position coordinate x also has its associated operator $\hat{x}$ defined by the operation

$$\hat{x}\Psi(x,t)=x\Psi(x,t) \tag{1.6.17}$$

Therefore $\hat{x}$ is a multiplication operator, i.e., when $\hat{x}$ operates on any function, the resultant is the multiplication of that function by x. For the sake of brevity, we can rewrite Eq.(1.6.17) as

$$\hat{x}=x \tag{1.6.18}$$

It is to be noted that $\hat{x}=x$ is only hold in explaining the equivalent operational effect of $\hat{x}$. In notation they stand for different meanings: $\hat{x}$ is a operator, while x is a physical quantity; an operator is never equal to a quantity.

The operator concept is useful in quantum mechanics because the expectation value $\langle Q\rangle$ of any observable Q can be expressed in terms of its associated operator $\hat{Q}$ as

$$\langle Q\rangle=\int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{Q}\Psi(x,t)dx \tag{1.6.19}$$

Several special cases of Eq.(1.6.19) are discussed in the following.

(1) $Q=x$:

$$\langle x\rangle=\int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{x}\Psi(x,t)dx=\int_{-\infty}^{+\infty}\Psi^*(x,t)x\Psi(x,t)dx=\int_{-\infty}^{+\infty}x\left|\Psi(x,t)\right|^2dx$$

This is the result already derived in Eq.(1.6.2).

(2) $Q=p$:

$$\langle p\rangle=\int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{p}\Psi(x,t)dx=\frac{\hbar}{i}\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}dx$$

This is the result already derived in Eq.(1.6.9).

(3) $Q=V(x)$:

$V(x)$ is potential energy which is only a function of position x, but not a function of p. Its expectation value can be obtained by setting $Q=V(x)$ in Eq.(1.2.2.19), leading to

$$\begin{aligned}\langle V(x)\rangle&=\int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{V}\Psi(x,t)dx=\int_{-\infty}^{+\infty}\Psi^*(x,t)V(\hat{x})\Psi(x,t)dx\\&=\int_{-\infty}^{+\infty}\Psi^*(x,t)V(x)\Psi(x,t)dx=\int_{-\infty}^{+\infty}V(x)\left|\Psi(x,t)\right|^2dx\end{aligned} \tag{1.6.20}$$

(4) $Q = K = p^2/2m$:
K is the kinetic energy whose associated kinetic energy operator $\hat{K}$ is defined via the relation

$$K = \frac{p^2}{2m} \quad \Rightarrow \quad \hat{K} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Its expectation value can be obtained by setting $Q = K$ in Eq.(1.6.19),

$$\begin{aligned}\langle K\rangle &= \int_{-\infty}^{+\infty}\Psi^*(x,t)\hat{K}\Psi(x,t)dx = \int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2\Psi(x,t)dx \\ &= -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\Psi^*(x,t)\frac{\partial^2\Psi(x,t)}{\partial x^2}dx\end{aligned} \tag{1.6.21}$$

(5) $Q = E = p^2/2m + V(x)$:
To find the average total energy $\langle E\rangle$, we sum the average kinetic and potential energy to get

$$\begin{aligned}\langle E\rangle &= \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(\frac{1}{2m}\hat{p}^2 + V(\hat{x})\right)\Psi(x,t)dx \\ &= \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t)dx = \int_{-\infty}^{+\infty}\Psi^*(x,t)\widehat{H}\Psi(x,t)dx\end{aligned} \tag{1.6.22}$$

where the operator $\widehat{H}$ is called Hamiltonian defined as

$$\widehat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{1.6.23}$$

In terms of $\widehat{H}$, the Schrodinger equation in Eq.(1.6.7)

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{1.6.24}$$

can be rewritten as

$$\widehat{H}\Psi(x,t) = \widehat{E}\Psi(x,t) \tag{1.6.25}$$

where $\widehat{E}$ is called energy operator defined as

$$\widehat{E} = i\hbar\frac{\partial}{\partial t} \tag{1.6.26}$$

Eq.(1.6.25) is the starting point of matrix mechanics which will be investigated in the next chapter. Table 1.6.2 summarizes several common observables and their associated operators. For every measurable quantity Q, there is an associated operator $\widehat{Q}$ in quantum mechanics. If wave function $\Psi(x,t)$ is determined, then the expectation value $\langle Q\rangle$ for any Q can be found from Eq.(1.6.19). This reveals the fact, as we have mentioned previously, that wave function provide all the information we need to describe the motion of a particle. The procedures of evaluating expectation are shown schematically in Fig.0.6.1.

1.6.4 Heisenberg Uncertainty Principle

Using expectation values, we can derive the Heisenberg uncertainty principle introduced in section 0.4. In quantum mechanics, uncertainty of a quantum variable is defined as the standard deviation of that variable. Hence according to the definition of standard deviation in Eq.(1.6.4), we have

$$\Delta x = \left\langle (x - \langle x\rangle)^2\right\rangle^{1/2}, \quad \Delta p = \left\langle \left(p - \langle p\rangle\right)^2\right\rangle^{1/2} \tag{1.6.27}$$

For the sake of simplicity in this derivation, we select $\langle x\rangle = \langle p\rangle = 0$ by assigning the origins of the position and momentum coordinates at time t to be the centers of the wave packet and its Fourier transform. With $\langle x\rangle = \langle p\rangle = 0$, Eq.(1.6.27) becomes

$$(\Delta x)^2 = \langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 \Psi^* \Psi dx = \int_{-\infty}^{+\infty} |x\Psi|^2 \, dx$$

$$(\Delta p)^2 = \langle p^2 \rangle = \left(\frac{\hbar}{i}\right)^2 \int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx = \left[\left(\frac{\hbar}{i}\right)^2 \Psi^* \frac{\partial \Psi}{\partial x}\right]_{-\infty}^{+\infty} - \left(\frac{\hbar}{i}\right)^2 \int_{-\infty}^{+\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} dx$$

$$= \int_{-\infty}^{+\infty} \left(\frac{-\hbar}{i} \frac{\partial \Psi^*}{\partial x}\right)\left(\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}\right) dx = \int_{-\infty}^{+\infty} \left|\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}\right|^2 dx$$

The product $(\Delta x \Delta p)^2$ is

$$(\Delta x \Delta p)^2 = \int_{-\infty}^{+\infty} |x\Psi|^2 \, dx \bullet \int_{-\infty}^{+\infty} \left|\frac{\hbar}{i} \frac{\partial \Psi}{\partial x}\right|^2 dx \tag{1.6.28}$$

The lower bound of $(\Delta x \Delta p)^2$ can be found by applying Schwartz's inequality:

$$\int |a(x)|^2 \, dx \bullet \int |b(x)|^2 \, dx \geq \left| \int a^*(x) b(x) dx \right|^2 \tag{1.6.29}$$

Also note $|z|^2 \geq |\mathrm{Im}\, z|^2$, and since $\mathrm{Im}\, z = (z - z^*)/2i$, we have $|z|^2 \geq \left|z - z^*\right|^2 / 4$. Letting $z = a^*(x)b(x)$ in the above equation, yields

$$\left|a^*(x)b(x)\right|^2 \geq \left|a^*(x)b(x) - a(x)b^*(x)\right|^2 / 4 \tag{1.6.30}$$

Combination of Eq.(1.6.29) and Eq.(1.6.30) gives

$$\int |a(x)|^2 \, dx \bullet \int |b(x)|^2 \, dx \geq \frac{1}{4} \left| \int \left[a^*(x)b(x) - a(x)b^*(x)\right] dx \right|^2 \tag{1.6.31}$$

Substituting $a(x) = x\Psi$ and $b(x) = (\hbar / i)\partial\Psi / \partial x$ into the above equation, we obtain

$$(\Delta x \Delta p)^2 \geq \frac{1}{4} \left| \frac{\hbar}{i} \int_{-\infty}^{+\infty} \left(x\Psi^* \frac{\partial \Psi}{\partial x} + x\Psi \frac{\partial \Psi^*}{\partial x} \right) dx \right|^2 = \frac{\hbar^2}{4} \left| \int_{-\infty}^{+\infty} x \frac{\partial}{\partial x} \left(\Psi^* \Psi\right) dx \right|^2$$

$$= \frac{\hbar^2}{4} \left| \left[x\Psi^* \Psi\right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \Psi^* \Psi dx \right|^2$$

The integrated part vanished because Ψ goes to zero faster than $1/\sqrt{x}$, as x approach $(\pm)$ infinity and the remaining integral is unity by the normalization condition of Ψ. Finally taking the square root, we obtain an explicit form of the Heisenberg uncertainty principle

$$\Delta x \Delta p \geq \hbar / 2 \tag{1.6.32}$$

This expression is consistent with the earlier form derived from the property of Fourier transformation, but here Eq.(1.6.32) is based on a precise definition of the uncertainty.

1.7 Particles in One-Dimensional Box

The central role of wave mechanics is played by the time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1.7.1}$$

where V is a given potential function. The solution of this equation provides us all the information we need to describe the motion of a particle. As the first application of this equation to a system with a specific form for $V(x)$, we consider a particle moving in a "box" potential.

An infinite square well has infinite height of potential at the points $x = 0$ and $x = L$, where L is the length of the box (refer to Fig.1.7.1(c)). Inside the box the particle is free; at the edges, however, it experiences strong forces that serve to contain it. A practical implementation of such a box is a

charged particle moving along the axis of aligned metallic tubes held at different potentials, as shown in Fig.1.7.1(a). The central tube is grounded, so that a test charge inside this tube has zero potential energy and experiences no electric force. When both outer tubes are held at a high electric potential V, there are no electric fields within them, but strong repulsive fields arise in the gaps at 0 and L. The potential energy $V(x)$ for this situation is sketched in Fig.1.7.1(b). As V is increased without limit and the gaps are simultaneously reduced to zero, we then approach the idealization known as the infinite square well or box potential:

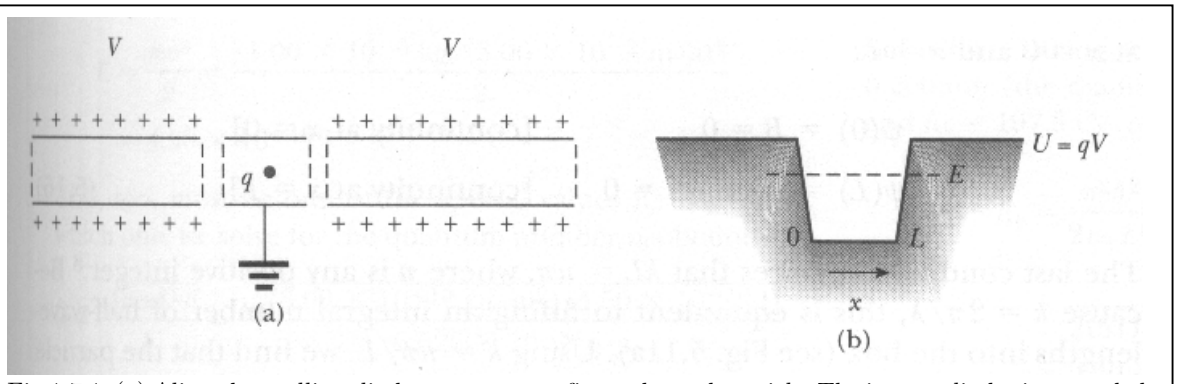

Fig.1.7.1. (a) Aligned metallic cylinders serve to confine a charged particle. The inner cylinder is grounded, while the outer ones are held at some high electric potential V. (b) The potential seen by this charge. (c) As V in increased and the gaps between cylinders are narrowed, the potential energy approaches that of the infinite square well.

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & x < 0,\ x > L \end{cases}$$

Substituting $V(x)$ into Eq.(1.7.1), we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \quad 0 \le x \le L \tag{1.7.2a}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \infty\psi = E\psi, \quad x > L,\ x < 0 \tag{1.7.2b}$$

The solution for Eq.(1.7.2b) is simply $\psi(x) = 0$, indicating that the probability is zero for finding the particle outside the box. Inside the box, Eq.(1.7.2a) becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi(x), \qquad k^2 = \frac{2mE}{\hbar^2} \tag{1.7.3}$$

The general solution is in the form of

$$\psi(x) = \begin{cases} A\sin kx + B\cos kx, & 0 \le x \le L \\ 0, & x > L,\ \ x < 0 \end{cases} \tag{1.7.4}$$

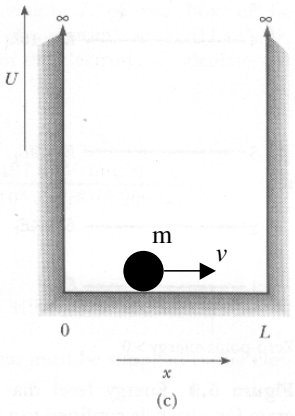

Fig.1.7.1. (c) Particle moving in a box with wall of infinite potential energy.

This interior wave must match the exterior wave at the walls of the box for $\psi(x)$ to be continuous everywhere. Thus, we require the interior wave to vanish at $x = 0$ and $x = L$:

$$\psi(0) = B = 0 \qquad \text{continuity at } x = 0 \tag{1.7.5a}$$

$$\psi(L) = A\sin kL = 0 \qquad \text{continuity at } x = L \tag{1.7.5b}$$

Eq.(1.7.5b) requires

$$kL = n\pi, \quad n = 1, 2, \cdots \tag{1.7.6}$$

Using $k = n\pi / L$ in Eq.(1.7.3), we find that the particle energies are quantized, being restricted to

the values

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2 h^2}{8mL^2}, \quad n = 1,2,\cdots \tag{1.7.7}$$

The lowest allowed energy, also called zero-point energy, is given by $n = 1$ and $E_1 = \pi^2\hbar^2 / 2mL^2$. Notice that $E = 0$ is not allowed; that is, the particle can never be at rest. This result clearly contradicts the classical prediction, for which $E = 0$ is an acceptable energy.

For the particle in a box, the uncertainty Δx in position is equal to the length L since the particle is somewhere within the box. The uncertainty Δp in momentum is equal to $2|p|$ since the momentum ranges from $-|p|$ to $|p|$. The momentum and energy are related by

$$|p| = \sqrt{2mE} = \frac{nh}{2L}$$

where the expression for E from Eq.(1.7.7) has been used. Hence,

$$\Delta x \bullet \Delta p = (L)(2|p|) = L\frac{2nh}{2L} = nh > \hbar / 2$$

is in agreement with the Heisenberg uncertainty principle. If the lowest allowed energy level were zero, then the Hensenberg uncertain principle would be violated.

With $k = n\pi / L$ and $B = 0$, the wave function in Eq.(1.7.4) becomes

$$\psi_n(x) = A\sin(n\pi x / L) \tag{1.7.8}$$

For each value of the quantum number n there is a specific wave function $\psi_n(x)$ describing the state of the particle with energy E_n. Fig.1.7.2 shows plots of $\psi_n(x)$ Versus x and of the probability density $|\psi_n|^2$ versus x for $n = 1,2,$ and 3, corresponding to the three lowest allowed energies for the particle. Inspecting Fig.1.7.2, we have the following observations:

(1) For $n = 1$, the probability of finding the particle is largest at $x = L/2$, which is the most probable position for a particle in this state.
(2) For $n = 2$, $|\psi|^2$ is a maximum at $x = L/4$ and $x = 3L/4$; both points are equally likely places for a particle in this state to be found.
(3) There are points within the box where it is impossible to find the particle. For $n = 2$, $|\psi|^2$ is zero at the midpoint, $x = L/2$; for $n = 3$, $|\psi|^2$ is zero at the points $x = L/4$, and $x = 3L/4$. <u>But how does our particle get from one place to another when there is no probability for its being at points in between ?</u> It is as if there were no path at all. Taking $n = 2$ as an example, when the particle initially appears at a point between $0 < x < L/2$, it will remain within this interval; no possibility is allowed for the particle to jump into the other interval $L/2 < x < L$.

Actual probability can be computed only after ψ_n is normalized, that is,

$$1 = \int_{-\infty}^{+\infty} |\psi_n(x)|^2\, dx = A^2\int_0^L \sin^2(n\pi x / L)\, dx = (A^2/2)\int_0^L \left[1 - \cos(2n\pi x / L)\right] dx = A^2 L / 2$$

Thus the normalization requires $A = \sqrt{2/L}$, and the normalized wave functions becomes

$$\psi_n(x) = \begin{cases} \sqrt{2/L}\sin(n\pi x / L), & 0 \le x \le L \\ 0 & x < 0, \quad x > L \end{cases}$$

If we integrate the product of two different wave functions $\psi_n(x)$ and $\psi_m(x)$ with $n \neq m$, we find that

$$\int_0^L \psi_n(x)\psi_m(x)\ dx = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\ dx = \frac{2}{\pi}\int_0^\pi \sin n\theta \sin m\theta\ d\theta = 0$$

This result may be combined with the normalization relation to give

$$\int_0^L \psi_n(x)\psi_m(x)\ dx = \delta_{nm}$$

where δ_{nm} is the Kronecker delata defined by $\delta_{nm} = 1$, as $n = m$, and $\delta_{nm} = 0$, as $n \neq m$. Functions that obey the above relation are orthonormal. Finally, the stationary states $\Psi(x,t)$ for the

particle in a one-dimensional box are given by

$$\Psi_n(x,t) = \sqrt{2/L}\sin\left(n\pi x/L\right)e^{-i\left(n^2\pi^2\hbar/2mL^2\right)t}$$

The most general solution is formed by the linear superposition of the above solution,

$$\Psi(x,t) = \sqrt{\frac{2}{L}}\sum_{n=1}^{N} C_n \sin\left(\frac{n\pi x}{L}\right)e^{-i\left(n^2\pi^2\hbar/2mL^2\right)t}$$

It is worth noting that although $\Psi_n(x,t)$ is stationary in the energy state E_n, the general solution $\Psi(x,t)$ is not stationary because $\left|\Psi(x,t)\right|$ is not independent of time. Actually, $\Psi(x,t)$ is in a mixed state comprising Ψ_1, Ψ_2, $\cdots$, and Ψ_n, for which energy is uncertain and no quantized phenomenon can be observed. This fact tells us that not every quantity in quantum mechanics is quantized.

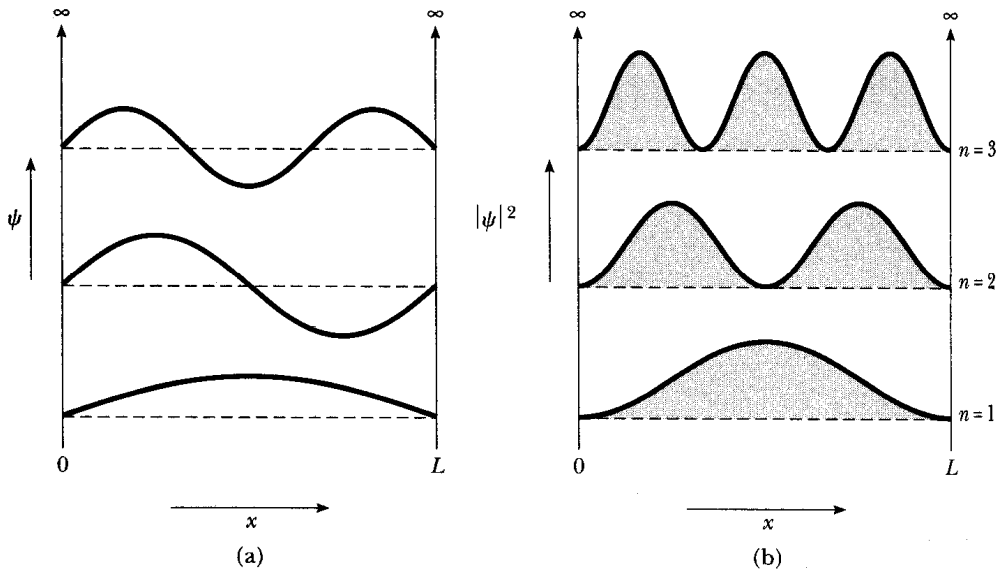

Fig.1.7.2. The first three allowed stationary states for a particle confined to a one-dimension box. (a) The wave functions for $n = 1,2,3$. (b) The probability density for $n = 1,2,3$.

Example 1.7.1

A particle is known to be in the ground state of an infinite square well with length L. Calculate the probability that this particle will be found within the interval $L/4 \le x \le 3L/4$.

Answer:

The probability density is given by $|\psi_1|^2$ for ground state, and the probability is

$$P = \int_{L/4}^{3L/4} |\psi_1(x)|^2\, dx = \frac{2}{L}\int_{L/4}^{3L/4} \sin^2(\pi x/L)\, dx$$

$$= \frac{1}{L}\int_{L/4}^{3L/4} \left[1-\cos(2\pi x/L)\right] dx = \left(\frac{1}{L}\right)\left[\frac{L}{2} - \left(\frac{L}{2\pi}\right)\sin(2\pi x/L)\right]_{L/4}^{3L/3} = 1/2 + 1/\pi \simeq 0.818$$

Note that this probability is considerably larger that 1/2, which would be expected for a classical particle spending equal time in all parts of the well.

1.8 Tunneling Phenomena

As the second application of Schrodinger equation, we consider the motion of a particle striking a potential barrier. Unlike potential wells that attract and trap particles, barriers repel them. Since barriers have no bound states, the main concern is to determine whether a particle incident on a barrier is reflected or transmitted. In the course of this study we shall encounter a peculiar phenomenon called tunneling, which is a purely wave-mechanical effect and is essential to the

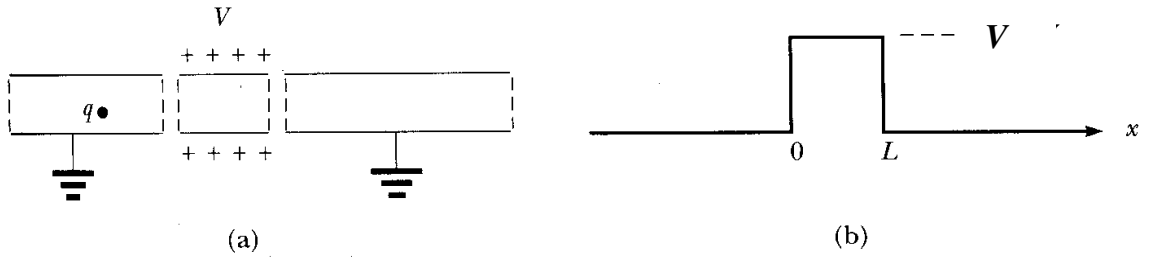

Fig.1.8.1 (a) Aligned metallic cylinders served as a potential barrier to charged particles. (b) The potential energy seen by this charge in the limit where the gaps between the cylinders have shrunk to zero size.

operation of many modern-day devices such as tunneling diode, scanning tunneling microscope (STM), laser and maser. In this section will discuss the role played by tunneling in several of these practical applications.

A square barrier is represented by a potential energy function $V(x)$ that is constant in the barrier region $0 \le x \le L$, and zero outside this region as shown in Fig.1.8.1(b). This square barrier can be realized by using charged hollow cylinders as shown in Fig.0.8.1(a), where the outer cylinders are grounded while the central one is held at some positive potential V . The charge experiences no force except in the gaps separating the cylinders. The force in the gaps is repulsive, tending to expel a positive charge q from the central cylinder.

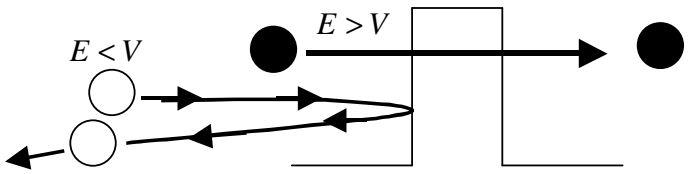

Fig.1.8.2. A classical particle incident on the barrier either reflects ($E < V$) or crosses the barrier $(E > V)$.

From the viewpoint of classical mechanics, the motion of a particle incident on the barrier can be described as following:

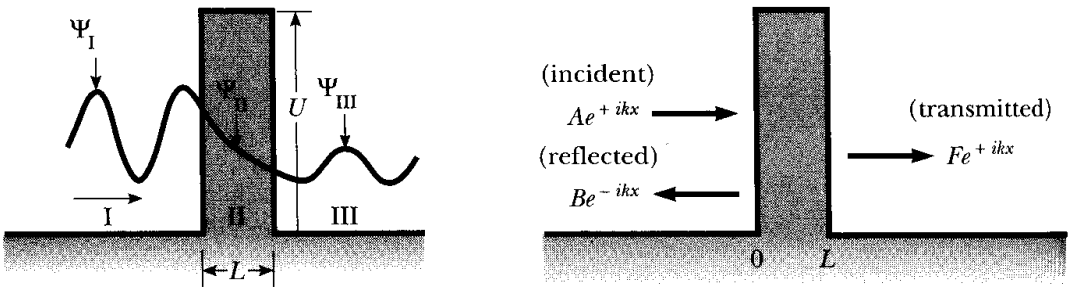

Fig.1.8.3. A typical wave function for a particle in the presence of a square barrier (left). The wave function is decomposed into incident, reflected, and transmitted waves (right).

(1) For a classical particle, with kinetic energy E greater than the potential height V , will experience a retarding force on arriving at $x = 0$, but is still able to overcome this force. On going into the barrier region, the particle will suffer a reduction in speed with the diminished kinetic energy $= E - V$. Such particles continue moving to the right with reduced speed until they reach $x = L$, where they receive a kick accelerating them back up to their original speed. Therefore, particles having energy $E > V$ are able to cross the barrier with their speed restored to the initial value.

(2) Particles with energy $E < V$ are turned back by the barrier, having insufficient energy to cross or penetrate it.

However, according to quantum mechanics there is no region inaccessible to the particle, regardless of its energy, since the wave function associated with the particle is nonzero everywhere. Even for a particle with $E < V$, there is a possibility for it to cross the barrier. This barrier penetration is in complete disagreement with classical physics. The attendant possibility of finding the particle on the far side of the barrier is called tunneling; we say that the particle has tunneled through the barrier. Time-independent Schrodinger equations for the three regions I, II, and III, shown in Fig.1.8.3, and their corresponding solutions are

$$\frac{d^2\psi}{dx^2} = \begin{cases} -\dfrac{2mE}{\hbar^2}\psi(x), & x < 0 \\ \dfrac{2m(V-E)}{\hbar^2}\psi(x), & 0 < x < L \\ -\dfrac{2mE}{\hbar^2}\psi(x), & x > L \end{cases} \quad \Rightarrow \quad \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{-\alpha x} + De^{\alpha x}, & 0 < x < L \\ Fe^{ikx} + Ge^{-ikx}, & x > L \end{cases} \tag{1.8.1}$$

where $k = \sqrt{2mE}\,/\,\hbar$ and $\alpha = \sqrt{2m(V-E)}\,/\,\hbar$. The physical meaning for each term in $\psi(x)$ is explained as follows:

(1) Ae^{ikx} stands for the wave moving from left to right in region I, and is interpreted as the wave incident on the barrier.

(2) Be^{-ikx} stands for the wave moving from right to left in region I, and is interpreted as the wave reflected from the barrier.

(3) Fe^{ikx} stands for the wave moving from left to right in region III, and is interpreted as the transmitted wave from the barrier.

(4) Ge^{-ikx} stands for the reflected wave moving from region III towards region II. But there is no potential barrier in region III, and G must be zero.

Based on the reflected wave Be^{-ikx} we can define the reflection coefficient R for the barrier as the ratio of the reflected probability density to the incident probability density:

$$R = \frac{\left(\Psi^*\Psi\right)_{\text{reflected}}}{\left(\Psi^*\Psi\right)_{\text{incident}}} = \frac{B^*B}{A^*A} = \frac{|B|^2}{|A|^2} = \left|\frac{B}{A}\right|^2 \tag{1.8.2}$$

In wave terminology R is the fraction of wave intensity in the reflected beam; in particle language, R becomes the probability that a particle incident on the barrier from the left is reflected by it.

Based on the transmitted wave Fe^{ikx} we can define the transmission coefficient T for the barrier as the ratio of the transmitted probability density to the incident probability density:

$$T = \frac{\left(\Psi^*\Psi\right)_{\text{transmitted}}}{\left(\Psi^*\Psi\right)_{\text{incident}}} = \frac{F^*F}{A^*A} = \frac{|F|^2}{|A|^2} = \left|\frac{F}{A}\right|^2 \tag{1.8.3}$$

Since a particle incident on the barrier is either reflected or transmitted, the probabilities for these events must sum to unity:

$$R + T = 1 \tag{1.8.4}$$

The reflection and transmission coefficients can be determined by substituting the following continuity requirements into Eq.(1.8.1):

(1) Continuity of ψ at $x = 0$: $A + B = C + D$ (1.8.5a)

(2) Continuity of $d\psi\,/\,dx$ at $x = 0$: $ikA - ikB = \alpha D - \alpha C$ (1.8.5b)

(3) Continuity of ψ at $x = L$: $Ce^{-\alpha L} + De^{+\alpha L} = Fe^{ikL}$ (1.8.5c)

(4) Continuity of $d\psi\,/\,dx$ at $x = L$: $\alpha De^{+\alpha L} - \alpha Ce^{-\alpha L} = ikFe^{ikL}$ (1.8.5d)

There are four equations that can be solved to find the four unknowns $B\,/\,A$, $C\,/\,A$, $D\,/\,A$, and $F\,/\,A$. After some manipulations, we obtain

$$T = \left|\frac{F}{A}\right|^2 = \left\{1 + \frac{1}{4}\left[\frac{V^2}{E(V-E)}\right]\sinh^2 \alpha L\right\}^{-1} \tag{1.8.6}$$

and the reflection coefficient is then found as $R = 1 - T$. A schematic plot of T versus E is shown in Fig.1.8.4, where it can be seen that $T(E)$ oscillates with E and transmission resonance occurs at E_1, E_2, and E_3, demonstrating evidence for the wave nature of matter.

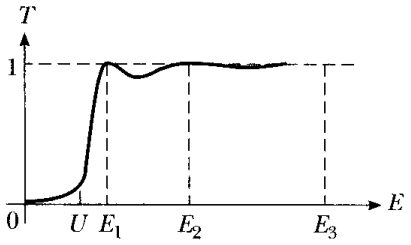

Fig.1.8.4. A schematic plot of the transmission coefficient T versus energy E

Example 1.8.1

Two copper conducting wires are separated by an insulating layer (CuO). Modeling the oxide layer as a square barrier of height 10.0eV, estimae the transmission coefficient for penetration by 7.00eV electrons: (a) if the layer thickness is 5.00nm, and (b) if the layer thickness is 1.00nm.

Answer :

To apply Eq.(1.8.6), α need be calculated first. Using $\hbar = 1.973\text{keV}\,\mathring{\text{A}}/\,\text{c}$, $m_e = 511\text{KeV}/\text{c}^2$ for electron to get

$$\alpha = \frac{\sqrt{2m_e(V-E)}}{\hbar} = \frac{\sqrt{2(511\text{keV}/\text{c}^2)(3.00\times10^{-3}\text{keV})}}{1.973\text{keV}\bullet\mathring{\text{A}}/\,\text{c}} = 0.8875\,\mathring{\text{A}}^{-1}$$

Using $L = 50.0\,\mathring{\text{A}} = 5.00\text{nm}$, $V = 10.0\text{eV}$ and $E = 7.00\text{eV}$, we obtain the transmission coefficient from Eq.(1.8.6)

$$T = \left\{1 + \frac{1}{4}\left[\frac{10^2}{7(3)}\right]\sinh^2(0.8875/\,\mathring{\text{A}})L\right\}^{-1} = 0.963\times10^{-38}$$

This is a fantastically small number. However, with $L = 10.0\,\mathring{\text{A}} = 1.00\text{nm}$, we find $T = 0.657\times10^{-7}$. Therefore, reducing the layer thickness by a factor of 5 enhances the likelihood of penetration by nearly 31 orders of magnitude !

1.9 Problems

1.1 Show that for a single particle with constant mass, the equation of motion implies the following differential equation for kinetic energy:

$$dT/\,dt = \boldsymbol{F}\bullet\boldsymbol{v}$$

while if the mass varies with time the corresponding equation is

$$d(mT)/\,dt = \boldsymbol{F}\bullet\boldsymbol{p}$$

1.2 Let q_1, q_2, $\cdots$, q_n be a set of independent generalized coordinates for a system of n degrees of freedom, with a Lagrangian $L(q,\dot{q},t)$. Suppose we transform to another set of independent coordinates s_1, s_2, $\cdots$, s_n by means of transformation equations

$$q_i = q_i(s_1, s_2, \cdots, s_n), \quad i = 1,2,\cdots,n\,.$$

Such a transformation is called point transformation. Show that if the Lagrangian function is expressed as a function of s_j, $\dot{s}_j$, and t through the equations of transformation, then L satisfies Lagrange's equations with respect to s coordinates:

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

In other words, the form of Lagrange's equation is invariant under a point transformation.

1.3 If L is a Lagrangian for a system of n degrees of freedom satisfying Lagrange's equations, show by direct substitution that

$$L'=L+dF(q_1,\cdots,q_n)/dt$$

also satisfies Lagrange's equations where F is any arbitrary, but differentiable, function of its arguments.

1.4 A particle of mass m moves in one dimensional such that it has the Lagrangian

$$L=(1/12)m^2\dot{x}^4+m\dot{x}^2V(x)-V^2(x)$$

where $V(x)$ is some differentiable function of x. Find the equation of motion for $x(t)$ and describe the physical nature of the system on the basis of this equation.

1.5 The term generalized mechanics has come to designate a variety of classical mechanics in which the Lagrangian contains time derivatives of q_i higher than the first. By applying the methods of the calculus of variation, show that if there is a Lagrangian of the form $L(q_i,\dot{q}_i,\ddot{q}_i,t)$, and Hamilton's principle holds with the zero variation of both q_i and $\dot{q}_i$ at the end points, then the corresponding Euler-Lagrange equations are

$$\frac{d^2}{dt^2}\left(\frac{\partial L}{\partial \ddot{q}_i}\right)-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)+\frac{\partial L}{\partial q_i}=0,\quad i=1,2,\cdots,n$$

Apply this result to the Lagrangian

$$L=-mq\ddot{q}/2-kq^2/2$$

Do you recognize the equations of motion ?

1.6 In certain situations, particularly one-dimensional systems, it is possible to incorporate frictional effects without introducing the dissipation function. As an example, find the equations of motion for the Lagrangian

$$L=e^{\gamma t}\left(m\dot{q}^2/2-kq^2/2\right)$$

How would you describe the system ? Are there any constants of motion ? Suppose a point transformation is made of the form $s=e^{\gamma t}q$. What is the effective Lagrangian in terms of s ? What do these results say about the conserved quantities for the system ?

1.7 On board an aircraft, a fire breaks out after landing. The passengers must leave by an emergency chute on which they glide down with friction. Determine by variational calculus the form of the chute with the aim to evacuate the plane as fast as possible. Assume the height of the hatch is y_0 and the distance to the bottom is x_0. Find the time of gliding as compared to the harsh free fall, assuming $x_0=(\pi/2)y_0$. This problem is known as the "brachistochrone" --- the curve of minimum time. Hint: First show that the gliding time is

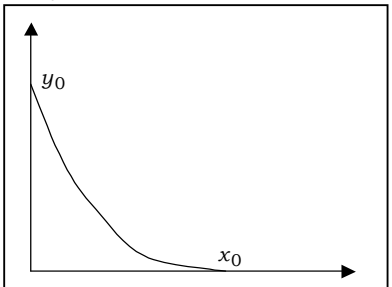

Fig.1.9.1 A Passenger glides down a chute

$$T=\int_0^T dT=\int_0^{x_0}\sqrt{\frac{1+(dy/dx)^2}{2g(y_0-y)}}dx$$

Then find the Euler-Lagrange equation for $y(x)$ minimizing the total time T. Solve the derived Euler-Lagrange equation by using the change of variable

$$y'=\frac{dy}{dx}=-\cot\frac{\theta}{2}$$

and show the curve of minimum time is represented by

$$x=(c^2/4g)(\theta-\sin\theta),\quad y=y_0-(c^2/4g)(1-\cos\theta)$$

from which, show the minimum time is

$$T=(\pi/2)\sqrt{2y_0/g}$$

1.8 In a region of space, a particle has a wavefunction $\psi(x) = Axe^{-x^2/L^2}$.
(a) Find the potential energy $V(x)$ as a function of x.
(b) Make a sketch of $V(x)$ versus x.

1.9 Consider a particle with energy E bound to a finite square well of height V and width $2L$ situated on $-L \le x \le L$.
(a) Show that for $E < V$, the conditions for smooth joining of the interior and exterior waves lead to the following equation for the allowed energies of the symmetric waves:

$$k \tan kL = \alpha \quad \text{(symmetric case)}$$

where $\alpha = \sqrt{(2m/\hbar^2)(V-E)}$, and $k = \sqrt{2mE/\hbar^2}$ is the wavenumber of oscillation in the interior.
(b) Show that the energy condition found in (a) can be rewritten as

$$k \sec kL = \sqrt{2mV}/\hbar$$

Apply the result in this form to an electron trapped at a defect site in a crystal, modeling the defect as a square well of height 5 eV and width 0.2 nm. Write a simple computer program to find the ground state energy for the electron. Give your answer accurate to ± 0.001 eV.

1.10 Which of the following functions are eigenfunctions of the momentum operator $\hat{p}_x$? What are their eigenvalues? (a) $A\sin(kx)$, (b) $A\sin(kx) - A\cos(kx)$, (c) $A\cos(kx) + iA\sin(kx)$, and (d) $Ae^{ik(x-a)}$

1.11 Consider a particle in an infinite square well described initially by a wave that is a superposition of the ground and first excited states of the well:

$$\Psi(x,0) = C\big(\psi_1(x) + \psi_2(x)\big)$$

(a) Show that the value $C = 1/\sqrt{2}$ normalizes this wave, assuming ψ_1 and ψ_2 are themselves normalized.
(b) Find $\Psi(x,t)$ at any later time t.
(c) Show that the superposition is not a stationary state, but that the average energy in this state is the arithmetic mean $(E_1 + E_2)/2$ of the ground and first excited state energies E_1 and E_2.
(d) Show that the average particle position $\langle x \rangle$ oscillates with time as

$$\langle x \rangle = x_0 + A\cos(\Omega t)$$

where

$$x_0 = \frac{1}{2}\left(\int x|\psi_1|^2\,dx + \int x|\psi_2|^2\,dx\right), \quad A = \int x\psi_1^*\psi_2 dx, \quad \Omega = (E_2 - E_1)/\hbar$$

Evaluate your results for the mean position x_0 and amplitude of oscillation A for an electron in a well 1 nm wide.

1.12 Particle incident on a potential step with a certain energy $E < V$ is described by the wave

$$\psi(x) = \begin{cases} \frac{1}{2}\big[(1+i)e^{ikx} + (1-i)e^{-ikx}\big], & x \le 0 \\ e^{ikx}, & x \ge 0 \end{cases}$$

(a) Verify by direct calculation that the reflection coefficient in unity in this case.
(b) How must k be related to E in order for $\psi(x)$ to solve Schrodinger's equation in the region to the left of the step ($x \le 0$)?
(c) Evaluate the penetration depth $\delta = 1/k$ for 10 MeV protons incident on this step.

1.13 Consider the scattering of particles from the potential well shown in Fig.1.9.2.
(a) Explain why the waves reflected from the well edges $x = 0$ and $x = L$ will cancel completely if $2L = \lambda_2$, where λ_2 is the de Broglie wavelength of the particle in region 2. This phenomenon is called perfect transmission.

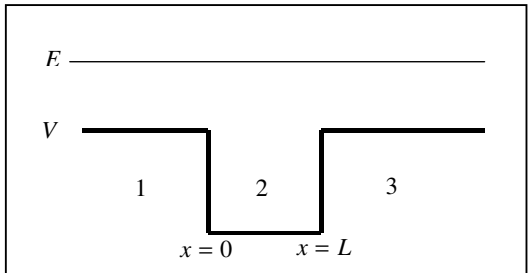

Fig.1.9.2 Potential well with $E > V$.

(b) Write expressions for the wave functions in regions 1, 2, and 3. Impose the necessary

continuity restrictions on Ψ and $\partial\Psi/\partial x$ to show explicitly that $2L = \lambda_2$ leads to no reflected wave in region 1.

This is a crude model for the Ramsauer- Townsend effect observed in the collisions of slow electrons with noble gases atoms like argon, krypton, and xenon. Electrons with just the right energy are diffracted around these atoms as if there were no obstacles in their path (perfect transmission). The effect is peculiar to the noble gases because their closed-shell configurations produce atoms with abrupt outer boundaries.

1.14 A particle of mass m moves in a three-dimensional box with edge length $L_1 = L$, $L_2 = 2L$, and $L_3 = 4L$. Find the energies of the ten lowest states and identify which of these are degenerate?

1.15 A particle of mass μ is fixed at one end of a rigid rod of negligible mass and length R. The other end of the rod rotates in the $x-y$ plane about a bearing located at the origin, whose axis is in the z direction. This two-dimensional "rigid rotator" is illustrated in Fig.1.9.3.

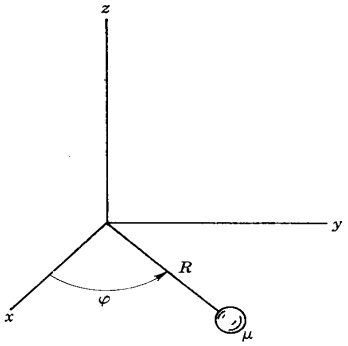

Fig.1.9.3 The rigid rotator moving in the $x-y$ plane considered in Problem 1.15.

(a) Write an expression for the total energy of the system in terms of is angular momentum L. (Hint: Set the constant potential energy to zero, and then express the kinetic energy in terms of L).

(b) By introducing the appropriate operators into the energy equation, convert it into the Schrodinger equation

$$-\frac{\hbar^2}{2I}\frac{\partial^2\Psi(\phi,t)}{\partial\phi^2} = i\hbar\frac{\partial\Psi(\phi,t)}{\partial\phi}$$

where $I = \mu R^2$ is the rotational inertia, or moment of inertia, and $\Psi(\phi,t)$ is the wavefunction. (Hint: Since the angular momentum is entirely in the z direction, $L = L_z$ and the corresponding operator is $\hat{L}_z = -i\hbar\partial/\partial\phi$).

(c) By applying the technique of separation of variables $\Psi(\phi,t) = \Phi(\phi)T(t)$, split the rigid rotator Schrodinger equation to obtain

$$-\frac{\hbar^2}{2I}\frac{d^2\Phi(\phi)}{d\phi} = E\Phi(\phi), \quad \frac{dT(t)}{dt} = -\frac{iE}{\hbar}T(t)$$

Solve the above equations and show that the separation constant E is the total energy.

(d) Show that a particular solution to the time-independent Schrodinger equation is

$$\Phi(\phi) = e^{im\phi}, \quad m = \sqrt{2IE/\hbar}$$

(e) Apply the single-value condition to the above particular solution and show that the allowed values of the total energy E are

$$E = \frac{\hbar^2 m^2}{2I}, \quad |m| = 0,\ 1,\ 2,\ 3,\ \cdots$$

(f) Normalize the function $\Phi(\phi) = e^{im\phi}$ found in part (e).

(g) Calculate the expectation values $\langle L\rangle$, $\langle L^2\rangle$, and $\Delta L = \left\langle (L - \langle L\rangle)^2 \right\rangle$.