CHAPTER III

FEYNMAN PATH INTEGRAL IN QUANTUM MECHANICS

In proceeding to evaluate the geometrical phase by path integral method, the basic ideas of constructing the Feynman path integral (Feynman, 1961) will be presented in this chapter. We present in this chapter the mathematical formulation of the quantum-mechanical transformation or the propagator, in the form of a path integral.

Feynman Propagator

If a particle moves from one point to another point there are many possible paths which the particle can take. In terms of classical mechanics, when we consider the particle as a point, there is a principle of least action which expresses the condition that determines a particular path from among all the possible paths. For simplicity, we will restrict ourselves to the case of a particle moving in one dimension. Thus the position at any time can be specified by a coordinate x, a function of time. By the path, we therefore mean a function x(t).

If a particle starts from the point x_a at an initial time t_a and goes to the final point x_b at time t_b, there will be many possible paths in which the particle can travel. For each path there exists the action S,

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t)\, dt, \qquad (1)$$

where L is the lagrangian for the system.

The principle of least action states that the particular path x(t) in which the particle can travel is that for which S is a minimum. That is to say, the value of S is unchanged in the first order if the path x(t) is slightly modified. This particular path x(t) is called the classical path.

Quantum mechanics deals with probabilities, that is, it states that we cannot specify the position of a particle, we can only know the probability of its being found in a given place. The probability that a particle will be found to have a path x(t) lying somewhere within the space time continuum is the absolute square of a probability amplitude. The probability amplitude is associated with the entire motion of a particle as a function of time, rather than simply with the position of the particle at a particular time. Thus when we consider the path by which the particles goes from a to b, we must specify how much each trajectory contributes to the probability amplitude K(b, a). It is not just the particular path of extreme action which contributes; rather, it is the case that all the paths contribute. The contribution $\emptyset$ [x(t)] from a single path depends on the classical action for that path in units of $\hbar$.

$$\emptyset[x(t)] = (\text{const})\exp\left[\frac{i}{\hbar}S\{x(t)\}\right]$$

The amplitude K(b,a), is thus the sum over all trajectories between the end points a and b of contributions $\emptyset$ [x(t)],

$$K(b,a) = \sum_{\substack{\text{over all} \\ \text{paths from a to b}}} \emptyset[x(t)]$$

$$K(b,a) = \sum_{\substack{\text{over all} \\ \text{paths from a to b}}} \text{const} \exp\left[\frac{i}{\hbar} S\{x(t)\}\right]. \quad (2)$$

We have thus described the physical ideas concerned in the construction of the amplitude for a particle to reach a particular point in space and time by closely following its motion in getting there. So if we want to find the probability amplitude of the particle going from a to b, we have to carry out the sum in Eq. (2). But the number of paths from a to b is infinite, so Eq. (2) is very difficult to work with. Another method and more efficient method of computing the sum over all paths will now be described.

We choose a subset of all paths by first separating the independent time into small interval, ε . This gives us a set of successive times $t_1, t_2, t_3, ...$ between the values t_a and t_b, where $t_{i+1} = t_i + \varepsilon$, At each time t_i we select some special point x_i and constructing a path by connecting all the points so selected to form a line. This process is shown in Fig. 1. It is possible to define a sum over all paths constructed in this manner by taking a multiple integral over all values of x_i for i between 1 and n-1, where

$$n\varepsilon = t_b - t_a, \quad t_0 = t_a, \quad t_n = t_b,$$

$$x_0 = x_a, \quad x_n = x_b$$

By using this method, Eq. (2) then becomes

$$K(b,a) \approx \int\int \cdots \int \text{const} \exp\left[\frac{i}{\hbar} S\{x(t)\}\right] dx_1 \, dx_2 \cdots dx_{n-1}. \tag{3}$$

We do not integrate x_0 or x_n because these are the fixed end points x_a and x_b. In order to achieve the correct measure, Eq. (3) must be taken in the limit $\varepsilon \rightarrow 0$ and some normalizing factor A^{-n} which depends on ε must be provided in order that the limit of Eq. (3) becomes

$$K(b,a) \approx \lim_{\varepsilon \to 0} \frac{1}{A} \int\int \cdots \int \text{const} \exp\left[\frac{i}{\hbar} S\{x(t)\}\right] \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{n-1}}{A} . \tag{4}$$

Eq. (4) can also be written in a less restrictive notation as

$$K(b,a) \approx N \int\int \cdots \int \text{const} \exp\left[\frac{i}{\hbar} S\{x(t)\}\right] D(\text{path})$$

This is called a path integral and the amplitude K(b,a) is known as the Feynman propagator.

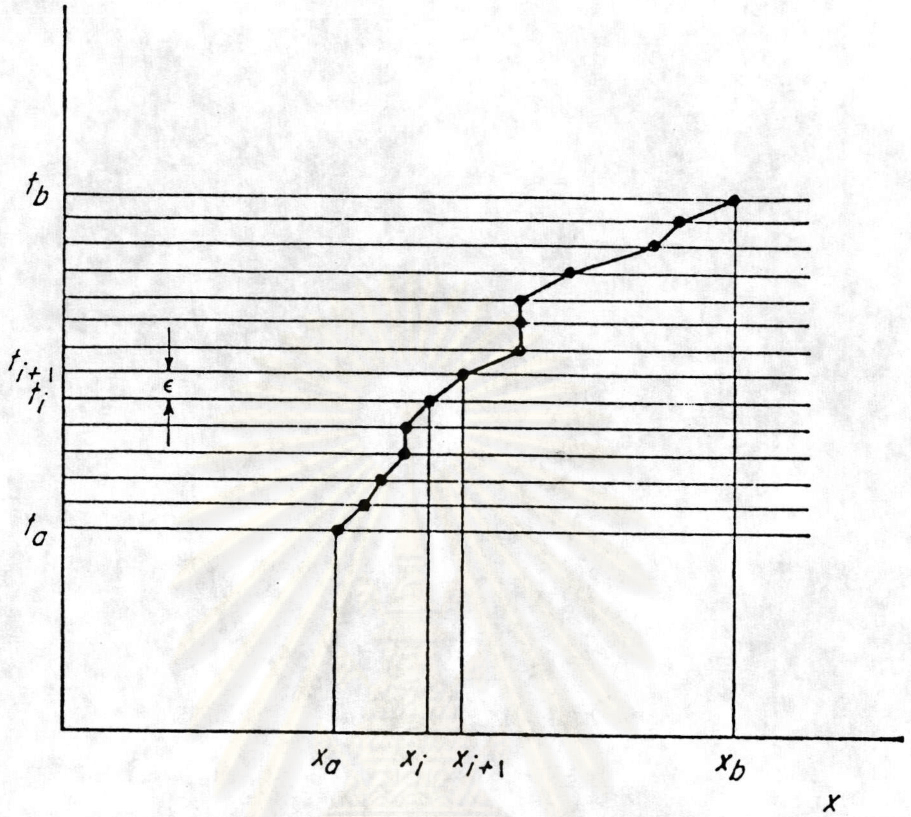

Fig. 1 Diagram showing how the path integrals can be constructed.

<u>Propagator from Schrödinger's Equation</u> (Schulman, 1981)

So far, we have followed Feynman's argument in writing down the propagator in the form of path integral. It will now be shown that the propagator in this form can also be derived directly from the Schrödinger's equation. The time-dependent Schrödinger's equation is

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] \psi(\mathbf{r}, t) = 0.$$

We can define the one-electron Green function of this equation as the solution of

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] G(\mathbf{r}, \mathbf{r}'; t, t') = \delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t').$$

Thus the Green function can be written as

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \left\langle \mathbf{r} \left| \exp\left\{ -\frac{i}{\hbar} \hat{H}(t - t') \right\} \right| \mathbf{r}' \right\rangle . \quad (5)$$

Let us divide the time interval $t - t'$ into n equal small subintervals, so that $t - t' = n\varepsilon$. By making use of the identity

$$\exp\left(-\frac{i\varepsilon\hat{H}n}{\hbar} \right) = \lim_{\varepsilon \to 0} \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right)^n ,$$

Eq. (5) becomes

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \lim_{\varepsilon \to 0} \left\langle \mathbf{r} \left| \underbrace{\left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right) \cdots \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right)}_{\text{n factor}} \right| \mathbf{r}' \right\rangle . \quad (6)$$

According to the rules of quantum mechanics we can insert a complete set of states between each pair of factors in Eq. (6):

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \lim_{\varepsilon \to 0} \int \int \cdots \int \left\langle \mathbf{r} \left| \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right) \right| \mathbf{r}_{n-1} \right\rangle d\mathbf{r}_{n-1}$$

$$\cdot \left\langle \mathbf{r}_{n-1} \left| \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right) \right| \mathbf{r}_{n-2} \right\rangle d\mathbf{r}_{n-2} \cdots$$

$$\cdot\, d\mathbf{r}_2 \left\langle \mathbf{r}_2 \left| \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right) \right| \mathbf{r}_1 \right\rangle d\mathbf{r}_1 \left\langle \mathbf{r}_1 \left| \left(1 - \frac{i\varepsilon\hat{H}}{\hbar} \right) \right| \mathbf{r}' \right\rangle \quad (7)$$

We now consider the Hamiltonian of the system in the position representation

$$\widehat{H} = \frac{p^2}{2m} + V(\mathbf{r}),$$

where p is the momentum operator. Then

$$\left\langle \mathbf{r}_{i+1} \left| \left(1 - \frac{i\varepsilon\widehat{H}}{\hbar} \right) \right| \mathbf{r}_i \right\rangle = \int \langle \mathbf{r}_{i+1} | \mathbf{p} \rangle d\mathbf{p} \left\langle \mathbf{p} \left| 1 - \frac{i\varepsilon}{\hbar} \left\{ \frac{p^2}{2m} + V(\mathbf{r}) \right\} \right| \mathbf{r}_i \right\rangle$$

$$= \int \langle \mathbf{r}_{i+1} | \mathbf{p} \rangle d\mathbf{p} \langle \mathbf{p} | \mathbf{r}_i \rangle \cdot \left[1 - \frac{i\varepsilon}{\hbar} \left\{ \frac{p^2}{2m} + V(\mathbf{r}) \right\} \right] \tag{8}$$

From quantum mechanics, the momentum eigenfunctions $\langle \mathbf{r} | \mathbf{p} \rangle$ for a free particle are

$$\langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left(\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right).$$

Therefore

$$\left\langle \mathbf{r}_{i+1} \left| \left(1 - \frac{i\varepsilon\widehat{H}}{\hbar} \right) \right| \mathbf{r}_i \right\rangle = \frac{1}{(2\pi\hbar)^3} \int \exp\left\{ \frac{i}{\hbar} (\mathbf{r}_{i+1} - \mathbf{r}_i) \cdot \mathbf{p} \right\} \cdot \left[1 - \frac{i\varepsilon}{\hbar} \left\{ \frac{p^2}{2m} + V(\mathbf{r}) \right\} \right] d\mathbf{p} \tag{9}$$

We now replace $1 - \frac{i\varepsilon}{\hbar}\left\{\frac{p^2}{2m} + V(\mathbf{r})\right\}$ by the corresponding exponential; the error introduced here is $O(\varepsilon^2)$, so that the total error from all the n factors can be neglected. Eq. (9) thus becomes

$$\left\langle \mathbf{r}_{i+1}\left|\left(1 - \frac{i\varepsilon\hat{H}}{\hbar}\right)\right|\mathbf{r}_i\right\rangle = \frac{1}{(2\pi\hbar)^3}\int \exp\left[-\frac{i\varepsilon}{\hbar}\left\{\frac{p^2}{2m} - \frac{(\mathbf{r}_{i+1} - \mathbf{r}_i)\cdot\mathbf{p}}{\varepsilon}\right\}\right]d\mathbf{p} \cdot \exp\left\{-\frac{i\varepsilon}{\hbar}V(\mathbf{r})\right\}$$

$$= \frac{1}{(2\pi\hbar)^3}\int \exp\left[-\frac{i\varepsilon}{2m\hbar}\left\{p^2 - \frac{2m(\mathbf{r}_{i+1} - \mathbf{r}_i)\cdot\mathbf{p}}{\varepsilon} + \left(\frac{m}{\varepsilon}(\mathbf{r}_{i+1} - \mathbf{r}_i)\right)^2 - \left(\frac{m}{\varepsilon}(\mathbf{r}_{i+1} - \mathbf{r}_i)\right)^2\right\}\right]d\mathbf{p} \cdot \exp\left\{-\frac{i\varepsilon}{\hbar}V(\mathbf{r})\right\}$$

$$= \frac{1}{(2\pi\hbar)^3}\int \exp\left[-\frac{i\varepsilon}{2m\hbar}\left\{\mathbf{p} - \frac{m}{\varepsilon}(\mathbf{r}_{i+1} - \mathbf{r}_i)\right\}^2\right]d\mathbf{p} \cdot \exp\left\{\frac{i\varepsilon}{2m\hbar}\left(\frac{m}{\varepsilon}(\mathbf{r}_{i+1} - \mathbf{r}_i)\right)^2\right\} \cdot \exp\left\{-\frac{i\varepsilon}{\hbar}V(\mathbf{r})\right\}$$

so

$$\left\langle \mathbf{r}_{i+1}\left|\left(1 - \frac{i\varepsilon\hat{H}}{\hbar}\right)\right|\mathbf{r}_i\right\rangle = \frac{1}{(2\pi\hbar)^3}\left(\frac{2m\pi\hbar}{i\varepsilon}\right)^{3/2} \cdot \exp\left\{\frac{im}{2\hbar\varepsilon}(\mathbf{r}_{i+1} - \mathbf{r}_i)^2 - \frac{i\varepsilon}{\hbar}V(\mathbf{r})\right\}$$

$$= \left(\frac{m}{2\pi\hbar i\varepsilon}\right)^{3/2} \exp\left[\frac{i\varepsilon}{\hbar}\left\{\frac{m}{2}\left(\frac{\mathbf{r}_{i+1}-\mathbf{r}_i}{\varepsilon}\right)^2 - V(\mathbf{r})\right\}\right] \tag{10}$$

Substituting for Eq. (10) in Eq. (7), we obtain

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \lim_{\varepsilon\to 0}\frac{1}{A}\int\int\cdots\int \exp\left[\frac{i\varepsilon}{\hbar}\sum_{i=0}^{n-1}\left\{\frac{m}{2}\left(\frac{\mathbf{r}_{i+1}-\mathbf{r}_i}{\varepsilon}\right)^2 - V(\mathbf{r})\right\}\right] \cdot\frac{d\mathbf{r}_1}{A}\frac{d\mathbf{r}_2}{A}\cdots\frac{d\mathbf{r}_{n-1}}{A} \tag{11}$$

where $\frac{1}{A} = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{3/2}$, $\mathbf{r}_n = \mathbf{r}$, $\mathbf{r}_0 = \mathbf{r}'$.

In an obvious notation

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \frac{1}{A}\int\int\cdots\int \exp\left[\frac{i}{\hbar}\int_{t'}^{t}\left\{\frac{m}{2}\dot{\mathbf{r}}^2 - V(\mathbf{r})\right\}dt\right] \cdot\frac{d\mathbf{r}_1}{A}\frac{d\mathbf{r}_2}{A}\cdots\frac{d\mathbf{r}_{n-1}}{A}\,. \tag{12}$$

It can be shown that the time-dependent Green function (11) of Schrödinger's equation has exactly the same form as the Feynman propagator (4). The latter can be written in this form by using the argument discussed at the beginning of this chapter. As a simple example of how to obtain $G(\mathbf{r}, \mathbf{r}'; t, t')$ written in the form of Eq. (12), let us consider the case of a free electron.

For a free electron $L = \frac{m}{2}\dot{\mathbf{r}}^2$, therefore by using Eq. (11), we obtain

$$G\left(\mathbf{r}, \mathbf{r}'; t, t'\right) = \lim_{\varepsilon \to 0} \frac{1}{A} \int \int \cdots \int \exp\left[\frac{i\varepsilon}{\hbar} \sum_{i=0}^{n-1} \frac{m}{2} \left(\frac{\mathbf{r}_{i+1} - \mathbf{r}_i}{\varepsilon} \right)^2 \right]$$

$$\cdot \frac{d\mathbf{r}_1}{A} \frac{d\mathbf{r}_2}{A} \cdots \frac{d\mathbf{r}_{n-1}}{A},$$

The calculation is carried out by direct integrations as follows:

Since $\displaystyle\int_{-\infty}^{\infty} \exp\left\{ a(\mathbf{r}_0 - \mathbf{r}_1)^2 + b(\mathbf{r}_2 - \mathbf{r}_1)^2 \right\} d\mathbf{r}_1$

$$= \left(-\frac{\pi}{a+b} \right)^{3/2} \exp\left\{ \frac{ab}{a+b} (\mathbf{r}_2 - \mathbf{r}_0)^2 \right\},$$

we have

$$\left(\frac{m}{2\pi i\hbar\varepsilon} \right)^3 \int_{-\infty}^{\infty} \exp\left\{ \frac{im}{2\hbar\varepsilon} \left[(\mathbf{r}_1 - \mathbf{r}_0)^2 + (\mathbf{r}_2 - \mathbf{r}_1)^2 \right] \right\} d\mathbf{r}_1$$

$$= \left(\frac{m}{2\pi i\hbar\varepsilon} \right)^3 \left(\frac{\pi i\hbar\varepsilon}{m} \right)^{3/2} \exp\left\{ \frac{im}{2\hbar(2\varepsilon)} (\mathbf{r}_2 - \mathbf{r}_0)^2 \right\}$$

$$= \left(\frac{m}{2\pi\hbar(2\varepsilon)} \right)^{3/2} \exp\left\{ \frac{im}{2\hbar(2\varepsilon)} (\mathbf{r}_2 - \mathbf{r}_0)^2 \right\}$$

Multiplying the result by $\left(\frac{2\pi i\hbar\varepsilon}{m} \right)^{-1/2} \exp\left\{ \frac{im}{2\hbar\varepsilon} (\mathbf{r}_3 - \mathbf{r}_2)^2 \right\}$ and integrating over $\mathbf{r}_2$,

we obtain

$$\frac{1}{A}\int\int \exp\left[\frac{im}{2\hbar\varepsilon}\left\{ (\mathbf{r}_1 - \mathbf{r}_0)^2 + (\mathbf{r}_2 - \mathbf{r}_1)^2 + (\mathbf{r}_3 - \mathbf{r}_2)^2 \right\}\right]\frac{d\mathbf{r}_1}{A}\,\frac{d\mathbf{r}_2}{A}$$

$$= \int \left(\frac{m}{2\pi i\hbar(2\varepsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar(2\varepsilon)}(\mathbf{r}_2 - \mathbf{r}_0)^2\right]$$

$$\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{3/2} \exp\left[\frac{im}{2\hbar\varepsilon}(\mathbf{r}_3 - \mathbf{r}_2)^2\right] d\mathbf{r}_2$$

$$= \left(\frac{m}{2\pi i\hbar(2\varepsilon)}\right)^{3/2}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{3/2}\left(\frac{-2\pi\hbar(2\varepsilon)}{3im}\right)^{3/2} \exp\left[\frac{im}{2\hbar(3\varepsilon)}(\mathbf{r}_3 - \mathbf{r}_0)^2\right]$$

$$= \left(\frac{m}{2\pi i\hbar(3\varepsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar(3\varepsilon)}(\mathbf{r}_3 - \mathbf{r}_0)^2\right].$$

In this way a recurring process is established by which, after (n-1) steps, we obtain

$$G_0\left(\mathbf{r}, \mathbf{r}'; t\right) = \left(\frac{m}{2\pi i\hbar n\varepsilon}\right)^{3/2} \exp\left[\frac{im}{2\hbar(n\varepsilon)}(\mathbf{r}_n - \mathbf{r}_0)^2\right]$$

since $n\varepsilon = t$, $\mathbf{r}_n = \mathbf{r}$ and $\mathbf{r}_0 = \mathbf{r}'$, therefore

$$G_0\left(\mathbf{r}, \mathbf{r}'; t\right) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \exp\left[\frac{im}{2\hbar t}(\mathbf{r} - \mathbf{r}')^2\right].$$

The method of direct integration can be carried out only for this simple case of a free electron. For other cases, the path integral is more difficult to work out.

In the next chapter, we will reviewed Kuratsuji and Iida's work , in context of the Born-Oppenheimer approximation, by the Feynman path integration method (Moody, Shapere, and Wilczek, 1989; Aitchison, 1987) .