Chapter 2

Feynman's Path Integral Theory

In this chapter, we will present Feynman's path integral method [8]. The path integral technique has been used to solve many problems such as polarons [28], polymers, and many fields of condensed matter physics, etc. In the first section, we will explain what the Feynman propagator is. Next, we will give some applications of Feynman's path integral approach on simple systems such as a free particle, a system with quadratic Lagrangian, and a harmonic oscillator [8]. Finally, we will give the physical and mathematical concepts about functional and functional derivatives.

2.1 Feynman's Propagator

In this section, the propagator [8] is explained in the context of the probability that a particle moves from one point to another point by many possible paths. We can consider the particle as a point in classical mechanics. The principle of least action expresses the condition that determines a particular path

$\bar{x}(t)$ of all the possible paths. For simplicity, we will restrict ourselves to the case of the particle moving in one dimension. So, the position at any time t can be specified by a coordinate x which is a function of time. A particle at an initial time t_a starts from the point x_a and then moves to the final point x_b at the final time t_b. We have the conditions that $x(t_a) = x_a$ and $x(t_b) = x_b$ for many possible paths in the area of interest. We can find, for each path, the action S from

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t)\, dt, \tag{2.1}$$

where L is the Lagrangian of the system. For a particle of mass m moving in a potential $V(x(t))$, which is a function of position x and time t, the Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 - V(x(t)). \tag{2.2}$$

In quantum mechanics, we cannot know exactly by which path the particle goes from x_a to x_b. Consequently, the total amplitude of going from x_a to x_b must be contributed by all paths. Feynman has found that they contribute equal amount to the total amplitude, but contribute at different phases. The phase of the contribution from a given path equals to $S/\hbar$. The probability $P(x_b, x_a)$ to go from x_a at the time t_a to x_b at the time t_b can be calculated by

$$P(x_b, x_a) = |K(x_b, x_a)|^2, \tag{2.3}$$

where $K(x_b, x_a)$ is a probability amplitude for a particle going from one point to another point during a finite time. This amplitude is the sum of contribution $\phi[x(t)]$ from all paths

$$K(x_b, x_a) = \sum_{over\ all\ paths\ from\ x_a\ to\ x_b} \phi[x(t)] \ , \tag{2.4}$$

where

$$\phi[x(t)] = (const) \exp\left[\frac{i}{\hbar} S[x(t)]\right] \ . \tag{2.5}$$

The phase is 2π of the ratio of the action $S[x(t)]$ along the path to Planck's constant. Therefore, from Eqs. (2.4) and (2.5), we get

$$K(x_b, x_a) = \sum_{over\ all\ paths\ from\ x_a\ to\ x_b} (const) \exp\left[\frac{i}{\hbar} S[x(t)]\right] \ . \tag{2.6}$$

Next, we select a subset of all paths from x_a to x_b. To do this, we divide the independent time into very small interval ϵ. This gives us a set of successive time intervals $t_1, t_2, t_3, ...$ between the initial time t_a and the end time t_b where $t_{i+1} = t_i + \epsilon$. At each time t_i we pick some special point x_i and construct a path by connecting all the points, then we set their forms to be a line. These processes are shown in Figure 2.1. It is possible to define a sum of overall paths constructed in this manner by taking a multiple integral over all values of x_i from i to $N-1$,

where

$$\left.\begin{array}{c} N\epsilon = t_b - t_a \\ \epsilon = t_{i+1} - t_i \\ t_0 = t_a \\ t_N = t_b \\ x_0 = x_a \\ x_N = x_b \end{array}\right\}. \tag{2.7}$$

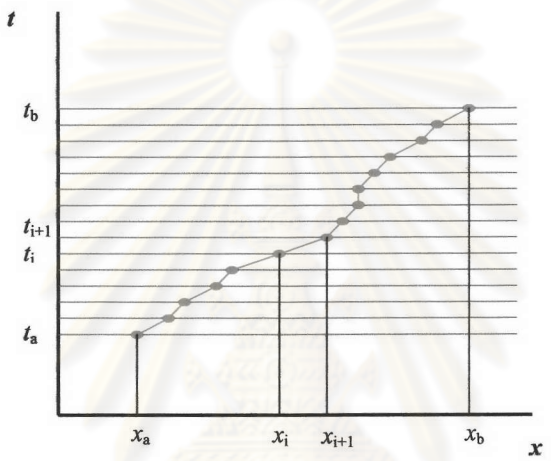

Figure 2.1 Diagram showing the sum over paths defined as a limit, in which at first the path is specified by giving only its coordinate x at a large number of specified times separated by very small interval ϵ. The path sum is then an integral over all these specific coordinates. Then to achieve the correct measure, the limit is taken as ϵ approaches zero [8].

Using the relation in Eq.(2.7) , we can write Eq. (2.6) as

$$K(x_b, x_a) \approx \int\int \ldots \int (const) \exp\left[\frac{i}{\hbar} S[x(t)]\right] dx_1\, dx_2 \ldots dx_{N-1}. \tag{2.8}$$

In the path integral, we do not consider integrate over x_0 or x_N because they are fixed end points. In order to achieve the correct measure, Eq. (2.8) must be taken in the limit of $\epsilon \to 0$. We must provide some normalizing factor A^{-N}. We find the right-hand side of Eq. (2.8) in the limit of $\epsilon \to 0$, so we obtain

$$K(x_b, x_a) = \lim_{\epsilon \to 0} \frac{1}{A} \int \int ... \int \exp\left[\frac{i}{\hbar} S[x(t)]\right] \frac{dx_1}{A} \frac{dx_2}{A} ... \frac{dx_{N-1}}{A}. \tag{2.9}$$

Finally we have

$$K(x_b, x_a) = \int \exp\left[\frac{i}{\hbar} S[x(t)]\right] D[x\,(t)], \tag{2.10}$$

where $D[x\,(t)]$ denotes the path-integration. The propagator in the above equation will be used to calculate the density of states for this work. More details about the path integrals can be found in Feynman and Hibbs' book [8].

2.2 Path Integral of a Free Particle

According to Eqs. (2.1) and (2.9), we now calculate the propagator of a free particle [8]. The Lagrangian for a free particle

$$L = \frac{1}{2} m \dot{x}^2. \tag{2.11}$$

According to Eq. (2.9) we can write

$$A = \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{\frac{1}{2}}. \tag{2.12}$$

From Eqs. (2.9) to (2.12) we can find the propagator for a free particle as

$$K(x_b, x_a) = \lim_{\epsilon \to 0} \int \int ... \int \exp\left[\frac{im}{2\hbar\epsilon} \sum_{i=1}^{N} (\vec{x}_i - \vec{x}_{i-1})^2\right] dx_i ... dx_{N-1} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{N}{2}}. \tag{2.13}$$

An integral of the form $\int_{-\infty}^{+\infty} dx \exp(-ax^2)$ or $\int_{-\infty}^{+\infty} dx \exp(-ax^2 + bx)$ is called a Gaussian integral. Since the integral of a Gaussian form is again a Gaussian, we may carry out an integration on one variable after another. The calculation is carried out as follows,

$$\int_{-\infty}^{+\infty} dx_1 \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{-\frac{3}{2}} \exp\left\{\left(\frac{m}{2\pi i\hbar\epsilon}\right)\left[(x_2 - x_1)^2 - (x_1 - x_0)^2\right]\right\}$$

$$= \left(\frac{m}{2\pi i\hbar(2\epsilon)}\right)^{\frac{1}{2}} \exp\left\{\frac{m}{2\pi i\hbar(2\epsilon)}(x_2 - x_0)^2\right\}. \tag{2.14}$$

After the integration is evaluated, the limit can be taken to obtain

$$K(x_b, x_a) = \left[\frac{2\pi i\hbar(t_b - t_a)}{m}\right]^{-\frac{1}{2}} \exp\left\{\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}\right\}. \tag{2.15}$$

2.3 The Quadratic Lagrangian

We have studied a simple example in the previous section. So, we shall now introduce some additional mathematical techniques which will help us to compute the sum over paths in certain situations. The simplest example to be studied is a quadratic Lagrangian [8] which corresponds to a case in which the

action S contains the path $x(t)$ up to the second power. To illustrate how the method works in such case, consider a particle whose Lagrangian has the form

$$L = a(t)\dot{x}^2(t) + b(t)\dot{x}(t)x(t) + c(t)x^2(t) + d(t)\dot{x}(t) + e(t)x(t) + f(t). \quad (2.16)$$

The action is the integral of this function with respect to times between two fixed end points. Actually, the Lagrangian in this form is a little more general than necessary. The factor $\dot{x}$ could be removed from those terms in which it is linear through an integration by parts. But this fact is unimportant for our present purpose. We wish to calculate the integral over all paths which go from (x_a, t_a) to (x_b, t_b)

$$K(x_b, x_a) = \int_{x_a}^{x_b} \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} L(\dot{x}, x, t)\right] D[x(t)]. \quad (2.17)$$

Certainly, it is possible to carry out this integral over all paths in the way that first described by dividing the region into short time elements, and so on. This follows from the fact that the integrand is the exponential of a quadratic form in the variable $\dot{x}$ and x. Such integrals can always be carried out. But we shall not go through this tedious calculation, since we can determine the most important characteristic of the kernel in the following manner. Let $\bar{x}(t)$ be the classical path between the specific end points. This is the path which has an extremum for the action S. In this thesis, we will use

$$S_{cl}[x_b, x_a] = S[\bar{x}(t)]. \quad (2.18)$$

We can represent x in terms of the classical path $\bar{x}(t)$ plus a new variable y: $x(t) = \bar{x}(t) + y(t)$. That is to say, instead of defining a point on the path by the displacement $x(t)$ from an arbitrary coordinate axis, we measure instead the deviation $y(t)$ from the classical path, as shown in Figure 2.2. Since any path $x(t)$ and the classical path $\bar{x}(t)$ must have the same end points. The condition which the derivations $y(t)$ have to satisfy is $y(t_a) = y(t_b) = 0$.

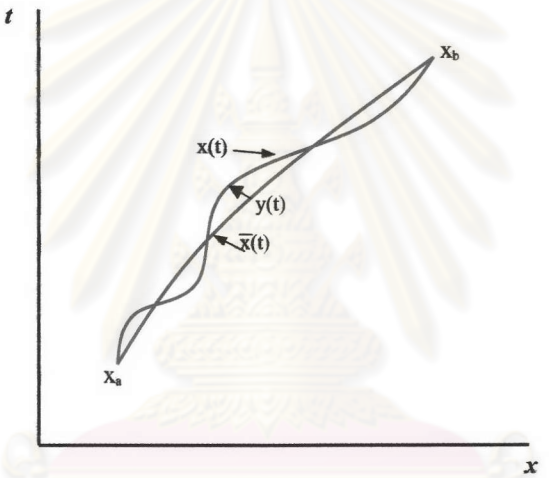

Figure 2.2 The difference between the classical path $\bar{x}(t)$ and some possible alternative path $x(t)$ is the function $y(t)$ [8].

Therefore, the action S can be expressed as

$$\begin{aligned} S[x(t)] &= S[\bar{x}(t) + y(t)] \\ &= \int_{t_a}^{t_b} \left[a(t) \left\{ \dot{\bar{x}}^2(t) + 2\dot{\bar{x}}\dot{y} + \dot{y}^2 \right\} + \ldots f(t) \right] dt. \end{aligned} \tag{2.19}$$

It is obvious that the integral of all terms involving exclusively $\bar{x}(t)$ is exactly the classical action and the integral of all terms, that are linear in $y(t)$, precisely vanishes from boundary condition. So, all the remaining terms in the integral are the second-order terms in $y(t)$ only. That is

$$S[x(t)] = S_{cl}[\bar{x}(t)] + \int_{t_a}^{t_b} \left[a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t) \right] dt. \tag{2.20}$$

Thus the propagator is the integral over paths $y(t)$ does not depend upon the classical path and all paths $y(t)$ start from and return to the point $y = 0$, can be written as

$$K(x_b, x_a) = N_0 \int_0^0 D[y(t)] \exp\left[\frac{i}{\hbar} \left(S_{cl}[\bar{x}(t)] + \int_{t_a}^{t_b} \left[a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t) \right] \right) \right]$$

$$= \exp\left\{ \frac{i}{\hbar} S_{cl}[\bar{x}(t)] \right\} N_0 \int_0^0 D[y(t)] \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left\{ a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t) \right\} \right], \tag{2.21}$$

where N_0 is a normalize factor. For the quadratic Lagrangian, the propagator can be written as

$$K(x_b, x_a) = F(t_b, t_a) \exp\left\{ \frac{i}{\hbar} S_{cl}[\bar{x}(t)] \right\}, \tag{2.22}$$

where the prefactor is

$$F(t_b, t_a) = N_0 \int_0^0 D[y(t)] \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left\{ a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t) \right\} \right]. \tag{2.23}$$

For the quadratic Lagrangian, it can be seen that the path integral in Eq. (2.21), which is a product of two functions, one of which does not depend upon the end point positions. This propagator is similar to the semi-classical approximation.

2.4 Path Integral of a Harmonic Oscillator

We consider the one-dimensional harmonic oscillator [8] of which the Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2. \tag{2.24}$$

We obtain the equation of motion by applying the Euler-Lagrange equation to the Lagrangian

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = 0. \tag{2.25}$$

Hence, we can write Eq. (2.25) as

$$\ddot{x} + \omega^2 x = 0. \tag{2.26}$$

We can see that the solution of Eq. (2.26) is

$$x(t) = A_0 \sin\omega t + B_0 \cos\omega t \tag{2.27}$$

where A_0 and B_0 are constants. From Eq. (2.27), we can use the boundary conditions $x(0) = x_1$ and $x(T) = x_2$. Then the constants A_0 and B_0 are

$$A_0 = \frac{x_2 - x_1 \cos\omega T}{\sin\omega T} \tag{2.28}$$

$$B_0 = x_1. \tag{2.29}$$

Eq. (2.27) thus becomes

$$x(t) = \frac{1}{\sin \omega T}[x_2 \sin \omega T + x_1 \sin \omega (T - t)]. \tag{2.30}$$

Then, the corresponding action can be expressed as

$$\begin{aligned} S_{cl}[\bar{x}(t)] &= \int_0^T \frac{m}{2}\left[\dot{\bar{x}}^2(t) - \omega^2 \bar{x}^2(t)\right] dt \\ &= \frac{m}{2}\left[\dot{\bar{x}}(T)\bar{x}(T) - \dot{\bar{x}}(0)\bar{x}(0) - \int_0^T \bar{x}(t)[\ddot{\bar{x}}(t) - \omega^2 \bar{x}\,(t)]dt\right]. \end{aligned} \tag{2.31}$$

Putting Eq. (2.26) into Eq. (2.31), we get

$$S_{cl}[\bar{x}(t)] = \frac{m}{2}\left[\dot{\bar{x}}(T)\bar{x}(T) - \dot{\bar{x}}(0)\bar{x}(0)\right]. \tag{2.32}$$

Using Eq. (2.30), we obtain

$$S_{cl}[\bar{x}(t)] = \frac{m\omega}{2\sin \omega T}\left[\cos \omega T(x_1^2 + x_2^2) - 2x_1 x_2\right]. \tag{2.33}$$

The prefactor associated with the propagator can be evaluated exactly. There by we have found that

$$F(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}}. \tag{2.34}$$

Finally, the time-independent propagator or the kernel of the harmonic oscillator is

$$K(x_b, x_a) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp\left\{\frac{im\omega}{2\hbar \sin \omega T}\left[\cos \omega T(x_1^2 + x_2^2) - 2x_1 x_2\right]\right\}. \tag{2.35}$$

2.5 Functional and Functional Derivative

We firstly consider a function $F(y)$. If we start at a point y_0 and move a distance dy, the function F changes by an amount

$$dF = F(y_0 + dy) - F(y_0) = F'(y)|_{y_0} dy. \tag{2.36}$$

For a function of several variables $F(y_1, y_2, y_3, ...)$, and its partial derivatives [8], $\frac{\partial F}{\partial y_1}, \frac{\partial F}{\partial y_2}, \frac{\partial F}{\partial y_3}, ...$ if one begins at a point $y_1^0, y_2^0, y_3^0, ...$ and moves to a new point via a displacement $dy_1, dy_2, dy_3, ...$,the function F will change by an amount

$$dF = \left.\frac{\partial F}{\partial y_1}\right|_{y_0} dy_1 + \left.\frac{\partial F}{\partial y_2}\right|_{y_0} dy_2 + \left.\frac{\partial F}{\partial y_3}\right|_{y_0} dy_3 + ... \tag{2.37}$$

If we write the independent variables $y_1, y_2, y_3, ...$ collectively as y_n $(n = 1, 2, 3, ...)$, y_n will look like a function of the integer variable n. F is thus a function of the function y. In physics, a function $y(x)$ usually depends on a variable x that takes on all real values in some interval $[a, b]$. This is related to what we have discussed so far, let's select N points on the interval $[a, b]$ with the points a distance ς apart, where $N\varsigma = b - a$. The n^{th} point is at $x = x_n = a + n\varsigma$. We can represent the function $y(x)$ by its value on the N point, so that we consider the function $y_n = y(x_n) = y(a + n\varsigma)$, which would give more and more information about the original $y(x)$ as $N \to \infty$, $\varsigma \to 0$. We can define a function of all the $\{y_n\}$, namely $F(\{y_n\})$. In the limit $N \to \infty$, the function F becomes a function of

the function $y(x)$. We then call F a functional of $y(x)$, written as $F[y]$. It is a function of all the values of $y(x)$ in the interval $[a,b]$: an infinite number of independent variables. A functional takes a function $y(x)$ on a domain as input not the value of the function at a specific point x, but all the values of y at all the $x's$ on the domain. Its output is a number. In case we change the values of $\{y_n\}$, the function $F(\{y_n\})$ will change according to Eq. (2.37). Now this equation can be written as

$$dF = \sum_{n=1}^{N} \left.\frac{\partial F}{\partial y_n}\right|_{y^0} dy_n. \tag{2.38}$$

Consider the limit $N \to \infty$. Recall that the definition of an integral is

$$\int_a^b dx f(x) = \lim_{\varsigma \to 0} \sum_{n=1}^{N} \varsigma f(x_n). \tag{2.39}$$

Eq. (2.38) can be written as

$$dF = \sum_{n=1}^{N} \varsigma \left(\frac{1}{\varsigma} \left.\frac{\partial F}{\partial y_n}\right|_{y^0} \right) dy_n. \tag{2.40}$$

Taking the limit $\varsigma \to 0$, with $x = a + n\varsigma$, and introducing the notation $dy_n = \delta y(x)$, the resulting Eq. (2.40) is

$$dF = \int_a^b dx \left.\frac{\delta F}{\delta y(x)}\right|_{y^0(x)} \delta y(x). \tag{2.41}$$

This $y^0(x)$, a particular function $y(x)$, is the starting point for the arbitrary infinitesimal change delta y of x. The $1/\varsigma$ has been absorbed into $\delta F/\delta y(x)$.

This can be taken to be the definition of the functional derivative $\delta F/\delta y(x)$. The meaning of Eq. (2.41) is exactly the same as the meaning of Eq. (2.40). The change in F is a sum of terms proportional to the infinitesimal changes $\delta y(x)$, with constants of proportionality that are just the functional derivative (i.e., the partial derivatives) $\delta F/\delta y(x)$. We can think of this derivative as giving the response of the functional F to a small change in y, with the change localized at x. The preceding discussion gives a definition of the functional derivative, but it does not give a useful method for calculating it since for each problem we would have to define carefully a mesh of points x_n and a function F of the discrete set $y(x_n)$. Usually, we have a functional $F[y]$, defined for functions y of a continuum variable x, and we need its functional derivative. We can start with Eq. (2.39) as a definition of the functional derivative. For example,

$$F[y] = \int_0^1 y^2(x)\,dx. \tag{2.42}$$

To calculate the functional derivative [8], we calculate the change dF that is due to an infinitesimal change $\delta y(x)$ in the independent variables

$$\begin{aligned} F[y+\delta y] &= \int_0^1 [y(x)+\delta y(x)]^2\,dx \\ &= \int_0^1 \left[y^2(x)+2y(x)\,\delta y(x)+\delta^2 y(x)\right]dx. \end{aligned} \tag{2.43}$$

Now we throw away $(\delta y)^2$, since δy is infinitesimal and we have $\delta y \to 0$ limit.

Thus to the first order in δy,

$$\begin{aligned} F[y+\delta y] &= \int_0^1 \left[y^2(x) + 2y(x)\,\delta y(x)\right] dx \\ &= F[y] + \int_0^1 2y(x)\,\delta y(x)\,dx. \end{aligned} \tag{2.44}$$

The infinitesimal change in F due to δy is thus

$$dF = F[y+\delta y] - F[y] = \int_0^1 2y(x)\,\delta y(x)\,dx. \tag{2.45}$$

Finally, we consider the crucial step of comparing Eq. (2.45) with Eq. (2.41). We thus identify

$$\frac{\delta F}{\delta y(x)} = 2y(x). \tag{2.46}$$

This is the prototype for all calculations of the functional derivative [8].