CHAPTER 3

Path Integral

In this Chapter, we shall introduce Feynman Path Integral method. This method represents the third formalism of Quantum Mechanics and can be expressed in the form of propagator. We will review basic idea in this method and use this method to calculate the free energy of the system.

3.1 Introduction

Early in 1940s, R.P. Feynman constructed another tool [1] for quantum mechanics. For a while, for simplicity, we shall restrict ourselves to the case of a particle moving in one dimension and specified by a position coordinate x, which is a function of time t. The trajectory starts from point x_a or a at an initial time t_a and goes to a final point x_b or b at a final time t_b or we can simply say that the particle goes from a to b. We shall have an amplitude, called a *kernel* or *propagator*, which we may write $K(b,a)$, to get from a to b. This will be the sum

[1] See original paper in Ref. [11] and text book in Ref. [12]

over all of the paths between points a and b. The path in classical mechanics so called the classical trajectory can be understood by the *principle of least action*. That is, there exists a certain action S which can be computed for each path. The real condition is that the action be an extremum. The action is given by the expression $S[b,a] = \int L(\dot{x},x,t)dt$ where L is the Lagrangian for the system. For a particle of mass m moving in a potential $V(x,t)$, which is a function of position and time, the Lagrangian is

$$L = \frac{m}{2}\dot{x}^2 - V(x,t). \tag{3.1}$$

The form of the extremum path is determined using procedures of the calculus of variations. The path is varied from the classical path with the condition that both end points are always fixed. Thus the extremum of variation satisfies the classical Lagrangian equation of motion

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{x}}) - \frac{\partial L}{\partial x} = 0. \tag{3.2}$$

Now we explain how each trajectory contributes to the total amplitude of all paths which go from a to b. They contribute equal amounts to the total amplitude, but contribute at different phases. The phase of the contribution from a given path is the action S for that path in units of the quantum of action $\hbar$. The probability $P(b,a)$ to go from a to b is the absolute square of the amplitude $K(b,a)$. This amplitude is the summation of the contributions $\phi[x(t)]$ from each path. The contribution of a path has a phase proportional to the action , then we have

$$K(b,a) \propto \sum_{\text{over all paths from } a \text{ to } b} \exp\{(i/\hbar)S[x(t)]\}. \tag{3.3}$$

In the classical limit, all paths contribute equally although their phase vary. The action is enormous in relation to $\hbar$ or we can say that $S \gg \hbar$ then, the phase $S/\hbar$ is a very large angle. If we move a small path on the classical scale, the change in the action is small too. These small changes in path will produce an enormous change in phase. The paths in a neighborhood cancel out the contribution. All the contributions from the paths in this region are nearly in phase and at phase, classical action S_{cl} do not cancel out. Therefore, only for paths in the vicinity of classical path can get important results. No particular trajectory is of overwhelming importance but we choose the classical path as a good approximation.

The summation of paths is analogous to the Riemann integral. We can follow through an analogous procedure. As shown in Fig. (3.1), we divide the independent variable time into steps of width ϵ. This gives us a set of values t_n spaced a distance ϵ apart between t_a and t_b. At each time t_n we select some special point x_n. We construct a path by connecting all the points. We take a multiple integral over all values of x_n for n between 1 and $N-1$, when we define $N\epsilon = t_b - t_a \equiv \tau$ where $\epsilon = t_{n+1} - t_n, t_0 = t_a, t_N = t_b, x_0 = x_a$ and $x_N = x_b$. The resulting equation is

$$K(b,a) \sim \int\int \ldots \int \phi[x(t)]\, dx_1\, dx_2 \ldots dx_{N-1}. \tag{3.4}$$

We obtain a more representative sample of the complete set of all possible paths a and b by making ϵ smaller but we cannot proceed to the limit of this process

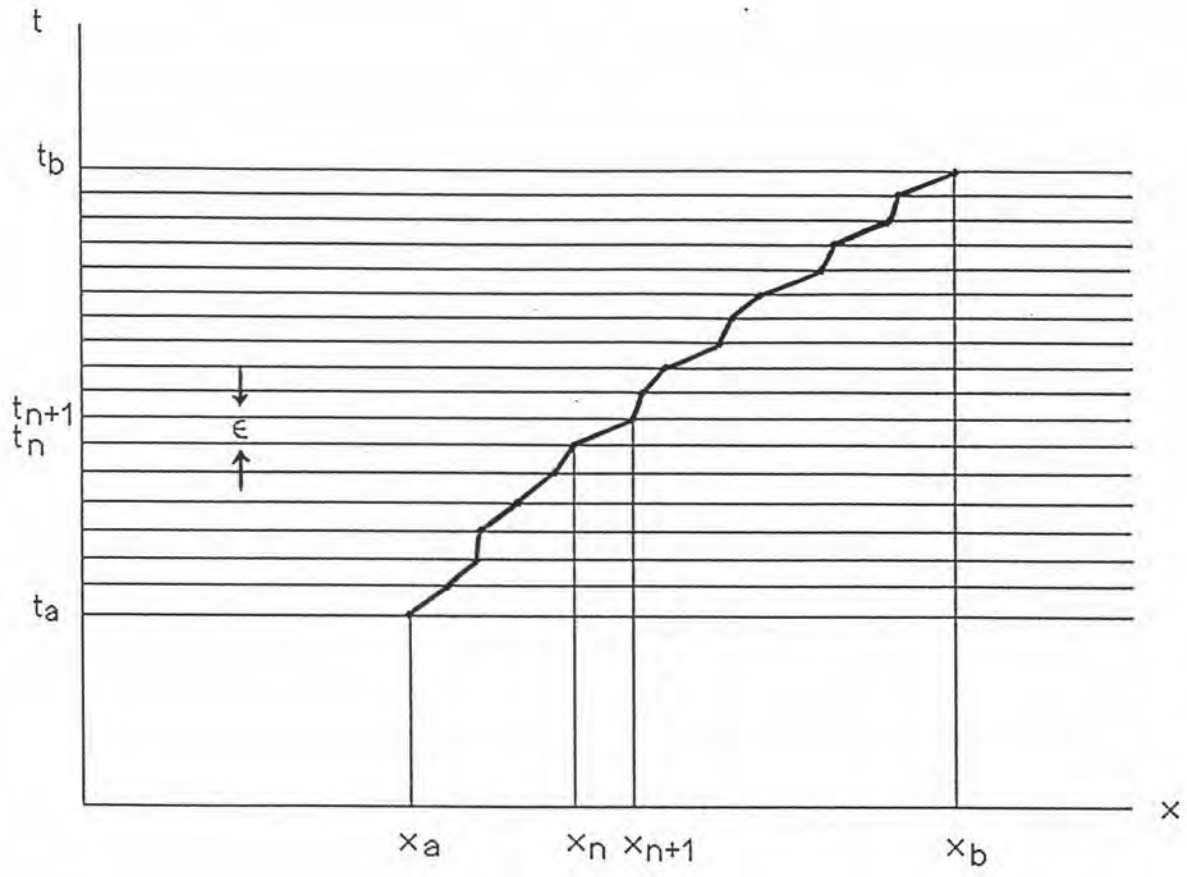

Figure 3.1: The sum over paths is defined as a limit, in which at first the path is specified by giving only its coordinate x at a large number of specified times separated by very small intervals ϵ. The path sum is then an integral over all these specific coordinates. Then to achieve the correct measure, the limit is taken as ϵ approach 0.

because the limit does not exist. Thus, we must provide some normalizing factor A for each path which depends on ϵ. Now the limit exists and the total amplitude going from a to b may be written as

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int \int \ldots \int e^{(i/\hbar)S[b,a]} \ \frac{dx_1}{A} \frac{dx_2}{A} \ldots \frac{dx_{N-1}}{A}. \tag{3.5}$$

For Eq. (3.5), we can find a normalized factor A by Ref. [12] in chap 4. We obtain $A = (2\pi i\hbar\epsilon/m)^{1/2}$. We shall write the sum over all paths in a short notation which is called a *path integral* as

$$K(b,a) = \int_a^b \ e^{(i/\hbar)S[b,a]} \ Dx(t). \tag{3.6}$$

3.2 Events in Succession

Now we have the problem of how to solve this expression of the path integral. What we need to know is the followings. We should know about events occurring in succession. To do this we must compose the amplitude for events which occur successively in time. If t_c is some time between t_a and t_b , we can show that the action along path between a and b can be written as $S[b,a] = S[b,c]+S[c,a]$. That is we can split any path into two parts and we then integrate them separately in three intervals, viz., integrating over all path from a to c in the first, from c to b in the second and the last at the point c. Thus

$$K(b,a) = \int_{x_c} K(b,c)K(c,a) \ dx_c \tag{3.7}$$

when we have many events, we can continue this process into N intervals. The result is

$$K(b,a) = \int_{x_1}\int_{x_2}\cdots\int_{x_{N-1}} K(b,N-1)\times$$
$$K(N-1,N-2)\ldots K(2,1)K(1,a)\; dx_1 dx_2 \ldots dx_{N-1}. \quad (3.8)$$

3.3 Relation with Wave Function

We have developed the amplitude for a particle to reach a particular point in space and time, however we can consider only the amplitude of arriving at a particular place without any data of the previous motion. We use the wave function $\psi(x,t)$ to represent this meaning since the wave function is an amplitude which corresponds to succession in time. We can apply Eq. (3.7) to the wave function to obtain

$$\psi(x_b,t_b) = \int K(x_b,t_b;x_c,t_c)\psi(x_c,t_c)dx_c. \quad (3.9)$$

We use the linear combinations of the steady-state functions $\phi_n(x)$, which are othonormal, to consider each state of the different energy level E_n. A wave function $\psi(x,t)$ can be expressed as $\sum_n c_n e^{-(i/\hbar)E_n t_b}\phi_n(x)$ where $c_n = e^{(i/\hbar)E_n t_a}\int \phi_n^*(x')\psi(x')dx'$. Substituting c_n in the wave function and rearranging, the wave function takes the form $\int(\sum_n \phi_n(x)\phi_n^*(x')e^{-(i/\hbar)E_n(t_b-t_a)})\psi(x')dx'$. We compare the integral term of this wave function to Eq. (3.9). We have the definition of the kernel in its wave function form as

$$K(x_b,t_b;x_a,t_a) = \sum_n \phi_n(x_b)\phi_n^*(x_a)e^{-(i/\hbar)E_n(t_b-t_a)}. \quad (3.10)$$

This expression for the kernel is very useful for translating expressions to more conventional representations. It expresses the kernel, which is originally a path integral, entirely in terms of solutions of the differential equation $H\phi = E\phi$.

3.4 Exact Solution

Next we proceed to a mathematical consideration of techniques to solve the kernel. This method is *Gaussian integrals.* The Lagrangian which corresponds to the action involving the path $x(t)$has the form $L(\dot{x}, x, t)$. All of the variables in an exponent might appear in second degree. For this reason, we can obtain an exact solution. This work follows the mathematical form that the integrand is an exponential of a quadratic form in the variables $\dot{x}$ and x. Let us specify the classical path $\bar{x}$ which represents an extremum of the action. From this path $x(t)$, we can consider separate paths to classical path $\bar{x}$ and variational δx. Then, we obtain the action $S[x(t)] = S[\bar{x} + \delta x] = S[\bar{x}] + S[\delta x]$ or we can separate the action in classical terms $S[\bar{x}]$ and the variational terms $S[\delta x]$.Then, considering the above two terms to be independent we can separate them. We have

$$K(b,a) = e^{\frac{i}{\hbar}S_{cl}[b,a]} \int_0^0 (\exp\{\frac{i}{\hbar}\int_{t_a}^{t_b} L(\delta\dot{x}, \delta x, t)dt\})\, D\delta x(t).$$

Since all paths $\delta x(t)$ start from and return to the point $\delta x = 0$, the integral over paths can be a function only of times at the end points. This means that the kernel can be written as

$$K(b,a) = e^{\frac{i}{\hbar}S_{cl}[b,a]} F(t_b, t_a) \tag{3.11}$$

where factor $F(t_b, t_a)$ represents the kernel in the variational or fluctuational terms. These factors can be found in the well-known formula of Van Vleck [13], Pauli [14] and Morette [15] which we call *Van Vleck-Pauli-Morette* formula. This formula [2] is

$$F(t_b, t_a) = (2\pi i\hbar)^{-(1/2)l} \left(Det_{\mu\nu}[\partial^2 S_{cl}[x_b, x_a]/\partial_\mu x_b \partial_\nu x_a \,]\right)^{1/2} \tag{3.12}$$

where l is the number of degrees of freedom or a dimensional space and $Det_{\mu\nu}$ is the determinant with respect to the indices μ and ν which are the parametric representation of a world line.

Suppose a system has several degrees of freedom such as $l = 2$. The system consists of a particle of mass m with x coordinate and the other system contains a particle of mass M with X coordinate. We shall discuss the two cases.

In the first case, these two systems interact with each other by a potential $V(x, X)$. The resulting action $S[x(t), X(t)]$ is $\int [(m/2)\dot{x}^2 + (M/2)\dot{X}^2 - V(x, X)]\, dt$ so that the kernel is

$$K(x_b, X_b, t_b; x_a, X_a, t_a) = \int_a^b \int_a^b \exp\{\frac{i}{\hbar} S[x(t), X(t)]\}\; Dx(t) DX(t). \tag{3.13}$$

Thus one might consider the motion of a point in some abstract two dimensional space with coordinates x and X. This kernel is the amplitude that the particle of mass m goes through from the point in space-time (x_a, t_a) to (x_b, t_b) and the particle of mass M goes from (X_a, t_a) to (X_b, t_b). The kernel is the sum of the amplitudes taken over all possible paths of both particles between their respective

[2] This formula can be proved in Ref. [15] by using events in succession idea.

end points. We solve this case by integrating over all of the variable functions but the analysis is very difficult. So we should use a *functional* which is a more powerful tool. Eq. (3.13) can be written as

$$K(b,a) = \int_a^b \exp\{(\frac{i}{\hbar}\int_{t_a}^{t_b} \frac{m}{2}\dot{x}^2 dt)\}\ T[x(t)]\ Dx(t) \tag{3.14}$$

where

$$T[x(t)] = \int_a^b \exp\{\frac{i}{\hbar}\int_{t_a}^{t_b}[\frac{M}{2}\dot{X}^2 + V(x,X,t)]dt\}\ DX(t). \tag{3.15}$$

Integrating over all paths to the X particle produces a functional $T[x(t)]$. The functional $T[x(t)]$ is the amplitude that the X particle goes along its end points under the influence of a potential V which depends upon both x and X. Assume that, x is held to a fixed path and X varies. So $V(x,X,t)$ is the potential of the X particle as the x particle moves along a specific trajectory. This amplitude depends on the trajectory of $x(t)$. Then, the total amplitude is obtained by summing over all paths of a functional consisting of the product of $T[x(t)]$ and the free-particle kernel for $x(t)$. The integral $T[x(t)]$ can be worked out or approximated for the possible values of the trajectory $x(t)$.

In the second case, if the action can be separated independently or we can say that the paricles do not interact, then $S[x,X] = S_x[x] + S_X[X]$ where S_x involves only the paths $x(t)$ and S_X involves only the paths $X(t)$. The kernel becomes the product of one factor depending on x and another depending on X alone. Thus

$$\begin{aligned} K(x_b,X_b,t_b;x_a,X_a,t_a) &= \int_a^b\int_a^b \exp\{\frac{i}{\hbar}(S_x[x]+S_X[X])\}Dx(t)DX(t) \\ &= \int_a^b \exp\{\frac{i}{\hbar}S_x[x]\}Dx(t)\ \int_a^b \exp\{\frac{i}{\hbar}S_X[X]\}DX(t) \end{aligned}$$

$$= K_x(x_b, t_b; x_a, t_a)\, K_X(X_b, t_b; X_a, t_a). \tag{3.16}$$

In a situation involving two independent noninteracting systems, the kernel for an event involving both systems is the product of two independent kernels.

3.5 Relation with Thermodynamics

In Chapter 2, the thermodynamic quantities can be represented in terms of the partition function and the free energy. Given both partition function and free energy it is possible to obtain all thermodynamic quantities. These quantities can be derived more generally by relating the propagator to the density matrix. In Chapter 4, it will be shown that the density matrix is related to the Feynman propagator by changing the real time into the imaginary time.