

## CHAPTER III

### FEYNMAN PATH INTEGRALS

The Feynman path integrals is a very powerful tool for solving many problems in quantum mechanics which is an alternative to the method of Heisenberg and Schrödinger. The purpose of this chapter is to explore Feynman's method of non-relativistic quantum mechanics. This method uses the knowledge about classical Lagrangians and the idea of probability amplitude.

#### Feynman Propagator

The concept of the amplitude of an event or the probability amplitude plays an important role in quantum mechanics. It is well known that quantum mechanics deals with probabilities, but the idea of the probability is not the whole picture in general, because the law of combining probabilities are not those of the classical probability theory of Laplace. In fact we have to use the concept of probability amplitude of an event where its absolute square is equal to the probability of that event., and the concept of the superposition of amplitude.

To discuss the Feynman's method, we shall limit ourselves to a one-dimensional problem, as the generalization of several dimension is obvious. Now supposing we have a particle of mass  $m$  which moves in one-dimensional space-time. At time  $t = t_a$  its coordinate is at  $x = x_a$ , and in the later time  $t = t_b$  it arrives at  $x = x_b$ . In general, the particle may be acted on by a potential  $V(x, t)$  which is the function of coordinate and time. It is well known that all information about the dynamical properties of the particle is contained in the classical action  $A[x(t)]$  which is

the functional of the path  $x(t)$ , and can be defined by the following equation<sup>[17][18]</sup>

$$A[x(t)] = \int_{t_a}^{t_b} L(\dot{x}, x, t) dt \quad (3.1)$$

where

$$L(\dot{x}, x, t) = \frac{1}{2} m \dot{x}^2 - V(x, t) \quad (3.2)$$

is the Lagrangian of the particle.

In classical mechanics, a particle will go to the final point from the initial point along the path which makes the action  $A[x(t)]$  in Eq.(3.1) minimum, known as the principle of least action, and this path is called the classical path. By use of the calculus of variation to vary the action in Eq.(3.1) which makes  $\delta A = 0$ , this leads to the classical equation of motion or Lagrange equation as

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0 \quad (3.3)$$

The solution of this equation is known as the classical path  $x_c(t)$  of the moving particle. By substituting the classical path into the Eq.(3.1), the result is the action  $A_c[x(t)]$  of classical path which is very useful to determine the propagator in Feynman path integral. At this point we have discussed the motion of the particle in the region of the classical theory, and know that it has a special path to move from one point to another point in space-time. But in quantum mechanics it is not correct. In quantum mechanics, it has many paths between two points which the particle can use in order to travel from one point to another point. Each of those paths has some probability amplitude associated with it. The probability amplitude of any path is a complex number where its absolute square is probability of that path; in addition, it has the assumption that the probability amplitude of each path has the same magnitude, but

different in phase which is equal to the action of that path in the unit of  $\hbar$ . If we represent the probability amplitude of the path  $x(t)$  by  $\phi[x(t)]$ , then

$$\phi[x(t)] = \text{const.} e^{(i/\hbar)A[x(t)]} \quad (3.4)$$

To sum of each  $\phi[x(t)]$  in Eq.(3.4) over all possible path  $x(t)$  one can get the total probability amplitude  $K(b,a)$  for the particle to move from the point labelled by  $a$  to the point  $b$ , and its absolute square,  $|K(b,a)|^2$ , shows the probability for the particle to move between these positions. We can write  $K(b,a)$  as follows

$$K(b,a) = \int_{x_a}^{x_b} \exp\left[\frac{i}{\hbar}A[x(t)]\right] Dx(t) \quad (3.5)$$

which we shall call a path integral. One can see that Eq.(3.5) shows the superposition of amplitude of all possible paths.

If we have a point  $(x_c, t_c)$  between two end points  $(x_a, t_a)$  and  $(x_b, t_b)$ , then we have

$$K(b,a) = \int_{x_c} K(b,c)K(c,a)dx_c \quad (3.6)$$

as the rule of the amplitude for events occurring in succession in time multiply. This property of propagator  $K$  is formally analogous to the Chapman-Kölmogolov equation satisfied by conditional probabilities of a Markoff process except that  $K$  here stands for the probability amplitude which is a complex number. For non-local actions which represent the memory effects, the above equation does not hold, but the path integral in Eq.(3.5) is still a meaningful concept and can be used to discuss the quantum mechanics of these actions.

The wave function  $\psi(x,t)$  has the meaning of the total amplitude for a particle

to arrive at  $(x, t)$  in space-time from the part in some situation, and its absolute square is the probability of finding the particle at the point  $(x, t)$  in space-time. We can see that  $K(x_b, t_b; x_a, t_a) = \psi(x_b, t_b)$  is actually a wave function, if we lose all knowledge of the particle at  $(x_a, t_a)$ . The propagator  $K(x_b, t_b; x_a, t_a)$  gives more information about the particle, in particular, that this is the amplitude for special case in which the particle came from  $(x_a, t_a)$ . So we can have the relation between  $\psi(x_b, t_b)$  and  $\psi(x_a, t_a)$  as following

$$\psi(x_b, t_b) = \int_{x_a} K(x_b, t_b; x_a, t_a) \psi(x_a, t_a) dx_a \quad \text{for } t_b > t_a. \quad (3.7)$$

This relation implies that

$$K(x_b, t_b; x_a, t_a) = \delta(x_b - x_a) \quad \text{for } t_a \rightarrow t_b. \quad (3.8)$$

For an infinitesimal time interval  $\varepsilon = t_b - t_a$ , one can show that the wave function  $\psi$  in Eq.(3.7) satisfies Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad (3.9)$$

where  $H$  is the Hamiltonian operator, and  $K$  must also satisfy a Schrödinger equation

$$i\hbar \frac{\partial K(b, a)}{\partial t_b} - H_b K(b, a) = 0 \quad \text{for } t_b > t_a \quad (3.10)$$

where  $H_b$  is a Hamiltonian operator operating on  $x_b$  only. The function  $K$  defined by a path integral in Eq.(3.5) is defined for  $t_b > t_a$ . The function is not defined for  $t_b < t_a$ , but with the help of following condition,

$$K(b, a) = 0 \quad \text{for } t_b < t_a \quad (3.11)$$

it is evident that Eq. (3.10) is also satisfied for  $t_b < t_a$ , but not for at the point  $t_b = t_a$  because  $K(b,a)$  is discontinuous at  $t_b = t_a$ . From the result of Eq.(3.8), the derivative of  $K(b,a)$  with respect to  $t_b$  gives a delta function in the time multiplied by  $\delta(x_b - x_a)$ . Hence  $K(b,a)$  satisfies

$$i\hbar \frac{\partial K(b,a)}{\partial t_b} - H_b K(b,a) = i\hbar \delta(x_b - x_a) \delta(t_b - t_a). \quad (3.12)$$

It is clear that the quantity  $K(b,a)$  is a kind of Green function for the Schrödinger equation  $\psi$  which satisfies the Schrödinger equation has the property  $\frac{d}{dt} (\int \psi^* \psi dx) = 0$ , the conservation of probability. By using this property and the relation in equation (3.8) we can show that

$$\int K^*(b, x'_a, t_a) K(b, x_a, t_a) dx_b = \delta(x'_a - x_a). \quad (3.13)$$

By multiplying equation (3.13) by  $K(a,c)$  and integrating  $x_a$ , then

$$\int K^*(b,a) K(b,c) dx_b = K(a,c) \quad (3.14)$$

where  $t_b > t_a > t_c$ .

When the classical Lagrangian has no explicit time dependence, the propagator can be expand to the following expansion

$$K(x_b, t_b; x_a, t_a) = \sum_n \exp[-\frac{i}{\hbar} E_n (t_b - t_a)] \psi_n^*(x_a) \psi_n(x_b), \quad (3.15)$$

say, in terms of a complete set of the energy eigenfunction  $\psi_n(x)$  of the Hamiltonian operator. This expansion is known as Feynman - Kac expansion theorem.<sup>[21]</sup>

### How to Calculate $K$

The previous section shows that the important quantity is the propagator  $K$ . In this section we shall introduce some techniques to calculate the propagator  $K$ , particularly, for the case of Lagrangian having the following form

$$L = \frac{I}{2} m \dot{x}^2 + V(x, t). \quad (3.16)$$

First, using the original construction of path integral introduced by Feynman as follows: consider a partition  $P_N$  of the time interval  $[t_a, t_b]$  into  $N$  subintervals which are of equal length, say  $\varepsilon$ , we characterize  $P_N$  by

$$\begin{aligned} P_N &: t_0 = t_a, t_1, t_2, \dots, t_{N-1}, t_N = t_b \\ t_j &= t_{j-1} + \varepsilon, N\varepsilon = t_b - t_a, \quad j = 1, 2, 3, \dots, N \end{aligned} \quad (3.17)$$

and the corresponding discretization of a path  $x(t)$  is

$$x_j = x(t_j), \quad x_a = x(t_0), \quad x_N = x(t_N) = x_b \quad (3.18)$$

This can say that at each time  $t_j$  we select some special point  $x_j$ , and then construct a path by connecting all the points so selected with straight lines. So the action  $A$  can be expressed in the discrete form as

$$A_N = \varepsilon \sum_{j=1}^N L \left( \frac{x_j - x_{j-1}}{\varepsilon}, \frac{x_j + x_{j-1}}{2}, \frac{t_j + t_{j-1}}{2} \right) \quad (3.19)$$

and the propagator  $K(b, a)$  can be rewritten as

$$K(b, a) = \lim_{\substack{\varepsilon \rightarrow 0 \\ N \rightarrow \infty}} \int \dots \int e^{i(\hbar)^{-1} A_N} \prod_{j=1}^{N-1} \frac{dx_j}{C^N} \quad (3.20)$$

To substitute  $u = T, T = t_b - t_a$  and taking the limit  $\epsilon \rightarrow 0$ , then

$$(3.25) \quad \left( \frac{2i\pi\hbar m \epsilon}{m} \right)^{L/2} \exp \left[ \frac{2i\pi\hbar m \epsilon}{m} (x_b - x_a) \right]$$

so after integrating any variables  $x_j, j = 1, 2, \dots, N-1$  we get  
 All integrations of this equation are Gaussian integrals, i.e., integrals of the form  $\int \exp(-ax^2 + bx)$ . Notice that the result of the Gaussian integral is again a Gaussian,

$$(3.24) \quad K(b, a) = \lim_{\epsilon \rightarrow 0} \left( \frac{2i\pi\hbar m \epsilon}{m} \right)^{L/2} \int \dots \int \exp \left[ \frac{2i\pi\hbar m \epsilon}{m} \sum_{j=1}^{N-1} (x_j - x_{j-1}) \right] \prod_{j=1}^{N-1} dx_j$$

Thus the propagator of the free particle is

$$(3.23) \quad A_N = \epsilon \sum_{j=1}^{N-1} \left( \frac{2i\pi\hbar m \epsilon}{m} \right)^{L/2} \int \dots \int dx_j$$

The action in discrete form is

$$(3.22) \quad L = \frac{1}{2} m \dot{x}^2$$

Let us consider a free particle of mass  $m$ , for example, which Lagrangian is

### i) The Free Particle

for the Lagrangian in form of Eq.(3.16). After integrating any variables of Eq.(3.16) and then taking the limit  $\omega \rightarrow 0$ , we shall get the propagator  $K$  for a problem concern.

$$(3.21) \quad C = \left( \frac{2i\pi\hbar m \epsilon}{m} \right)^{L/2}$$

where  $C$  is a normalizing factor, and

$$K(b, a) = \left( \frac{m}{2i\pi\hbar T} \right)^{1/2} \exp \left[ \frac{im}{2\hbar T} (x_b - x_a)^2 \right] \quad (3.26)$$

which is the propagator of a free particle.

For the Gaussian path integrals, all of the variables appear up to the second degree in an exponent, it has some mathematical techniques which help to compute the sum over all paths in certain situations. To make the discussion more definite, consider a particle with Lagrangian form

$$L = a(t)\dot{x}^2 + b(t)\dot{x}x - c(t)x^2 + d(t)\dot{x} + e(t)x + f(t) \quad (3.27)$$

and the action

$$A = \int_{t_a}^{t_b} [a(t)\dot{x}^2 + b(t)\dot{x}x - c(t)x^2 + d(t)\dot{x} + e(t)x + f(t)] dt \quad (3.28)$$

We wish to determine

$$K(b, a) = \int_a^b e^{i/\hbar A[x(t)]} Dx(t) \quad (3.29)$$

the integrals which go from  $(x_a, t_a)$  to  $(x_b, t_b)$ . Let  $x_c(t)$  be the classical path between the specified end points. The classical path  $x_c(t)$  is obtained from the Hamiltonian's principle. We have been using  $A_c$  stands for  $A[x_c(t)]$  the action of classical path which is extremum. Any paths  $x(t)$  can be expressed in term of  $x_c(t)$  and a deviation  $\eta(t)$  from  $x_c(t)$  as

$$x(t) = x_c(t) + \eta(t) \quad (3.30)$$

with the condition

$$\eta(t_a) = 0 = \eta(t_b) \quad (3.31)$$



Inserting Eq.(3.30) in Eq.(3.28), we get

$$A = \int_{t_a}^{t_b} [a\dot{x}_c^2 + b\dot{x}_c x_c + cx_c^2 + d\dot{x}_c + ex_c + f] dt + \int_{t_a}^{t_b} [a\dot{\eta}^2 + b\dot{\eta}\eta + c\eta^2] dt \\ + \int_{t_a}^{t_b} [(2a + bx_c d)\dot{\eta} + (b\dot{x}_c + 2cx_c + e)\eta] dt \quad (3.32)$$

the classical path  $x_c(t)$  must satisfy the Lagrange equation. So the equation of motion for the Lagrangian  $L$  in Eq.(3.28) is

$$2 \frac{d}{dt} (a\dot{x}) + (\dot{b} - 2c)x + \dot{d} - e = 0. \quad (3.33)$$

Considering the last integral in the right hand side of Eq.(3.32), we integrate  $\dot{\eta}(t)$  in this integral by parts then using Eq.(3.33), this integral vanishes. Notice that the first integral in Eq.(3.32) is the action  $A_c$ , so we can rewrite  $A$  as follows

$$A = A_c + \int_{t_a}^{t_b} [a\dot{\eta}^2 + b\dot{\eta}\eta + c\eta^2] dt \quad (3.34)$$

Since at the time  $t$  the quantity  $\eta(t)$  differ from  $x(t)$  only constant  $x_c(t)$ , so  $Dx(t) = D\eta(t)$ . Hence the propagator  $K$  can be written in the form

$$K(b, a) = F(t_b, t_a) e^{i/\hbar A_c} \quad (3.35)$$

when

$$F(t_b, t_a) = \int_{\eta(t_a)=0}^{\eta(t_b)=0} \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} [a\dot{\eta}^2 + b\dot{\eta}\eta + c\eta^2] dt \right\} D\eta(t) \quad (3.36)$$

Eq.(3.35) is very powerful to calculate  $K$  which the form of the Lagrangian is Eq (2.27). This is because it is not difficult to calculate the term classical action  $A_c$ , and the prefactor  $F(t_b, t_a)$  can be evaluated as follows

$$I(t_b, t_a) = \left( \frac{I}{2i\pi\hbar} \right)^{1/2} \left( -\frac{\partial^2 A_c}{\partial x_b \partial x_a} \right)^{1/2} \quad (3.37)$$

Actually, the propagator which is expressed in the form

$$K(b, a) = \left( \frac{I}{2i\pi\hbar} \right)^{1/2} \left( -\frac{\partial^2 A_c}{\partial x_b \partial x_a} \right)^{1/2} e^{(i/\hbar)A_c} \quad (3.38)$$

is called the Van Vleck-Pauli formula. We may use other techniques to evaluate the prefactor, for instance, expand Eq.(3.36) in terms of Fourier series we can also evaluate the terms prefactor.

## ii ) Harmonic oscillator

A Lagrangian of a harmonic oscillator is

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 \quad (3.39)$$

with the boundary condition  $x(t_a) = x_a$  and  $x(t_b) = x_b$ . By using Lagrange equation, the equation of motion for the harmonic oscillator is in the form

$$\ddot{x} + \omega^2 x = 0 \quad (3.40)$$

A solution of this equation, the classical path  $x_c(t)$ , which is subject to the boundary condition above, is of the form

$$x_c(t) = \frac{I}{\sin(\omega t)} \left[ x_a \sin \omega(t_b - t) + x_b \sin \omega(t - t_a) \right] \quad (3.41)$$

Inserting  $x_c(t)$  in Eq.(3.41) to Eq.(3.39), and taking the time integral from  $t_a$  to  $t_b$ , we can find  $A_c$  as

$$A_c = \frac{m\omega}{2 \sin \omega T} \left[ (x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right]. \quad (3.42)$$

Using Eq.(3.37) we find that

$$I(t_b, t_a) = \left( \frac{m\omega}{2i\pi\hbar \sin \omega T} \right)^{1/2}. \quad (3.43)$$

Thus, inserting Eq.(3.42) and (3.43) into Eq.(3.38), the propagator  $K(b, a)$  of a harmonic oscillator is

$$K(b, a) = \left( \frac{m\omega}{2i\pi\hbar \sin \omega T} \right)^{1/2} \exp \left\{ \frac{im\omega}{2\hbar \sin \omega T} \left[ (x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right] \right\}. \quad (3.44)$$

### iii) Forced harmonic oscillator

Supposing that the harmonic oscillator (the sub-section ii) is driven by an external force  $f(t)$ . The Lagrangian is

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 - f(t)x \quad (3.45)$$

The equation of motion is

$$\ddot{x} + \omega^2 x = -\frac{f}{m} \quad (3.46)$$

with boundary condition  $x(t_a) = x_a$  and  $x(t_b) = x_b$ , its solution is

$$\begin{aligned} x_c(t) = & x_a \frac{\sin \omega(t_b - t)}{\sin \omega T} + x_b \frac{\sin \omega(t - t_a)}{\sin \omega T} \\ & - \frac{1}{m\omega \sin \omega T} \int_{t_a}^{t_b} ds \left[ \Theta(s - t) \sin \omega(t_b - s) \sin \omega(t - t_a) \right. \\ & \left. + \Theta(t - s) \sin \omega(t_b - t) \sin \omega(s - t_a) \right] f(s) \end{aligned} \quad (3.47)$$

where  $\Theta(t)$  is the Heaviside step function which is unity for  $t \geq 0$  and zero for otherwise. The classical action for  $x_c(t)$  is

$$S_c = \frac{m\omega}{2 \sin \omega T} \left[ \int (x_a^2 + x_b^2) \cos \omega t' - 2x_a x_b - \frac{2x_b}{m\omega} \int_{t_a}^{t_b} dt f(t) \sin \omega(t - t_a) - \frac{2x_a}{m\omega} \int_{t_a}^{t_b} dt f(t) \sin \omega(t_b - t) - \frac{2}{m^2 \omega^2} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} ds f(t) f(s) \sin \omega(t_b - t) \sin \omega(s - t_a) \right]. \quad (3.48)$$

The prefactor  $F(t_b, t_a)$  is

$$F(t_b, t_a) = \left( \frac{m\omega}{2i\pi\hbar \sin \omega T} \right)^{1/2}. \quad (3.49)$$

The propagator is

$$K(b, a) = \left( \frac{m\omega}{2i\pi\hbar \sin \omega T} \right)^{1/2} \exp \left( \frac{im\omega}{2\hbar \sin \omega T} \left[ \int (x_a^2 + x_b^2) \cos \omega t' - 2x_a x_b - \frac{2x_b}{m\omega} \int_{t_a}^{t_b} dt f(t) \sin \omega(t - t_a) - \frac{2x_a}{m\omega} \int_{t_a}^{t_b} dt f(t) \sin \omega(t_b - t) - \frac{2}{m^2 \omega^2} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} ds f(t) f(s) \sin \omega(t_b - t) \sin \omega(s - t_a) \right] \right). \quad (3.50)$$

### Statistical Mechanics

Now it is appropriate to point out explicitly the significance of the Feynman path integral in a study of quantum statistical mechanics.<sup>[2],[3]</sup> The quantity important in solving statistical mechanical problems is density matrix, the average of states which describes the system over all ensemble.

We start this section by discussing briefly about density matrix as follow : Any system can be described by a density matrix  $\rho$ , where  $\rho$  is defined by

$$\rho = \sum_i w_i |\varphi_i\rangle\langle\varphi_i| \quad (3.51)$$

where  $|\varphi_i\rangle$  is an eigenket and its set forms a complete orthonormal set, and  $w_i$  is defined as follows

$$w_i \geq 0 \quad \text{and} \quad \sum_i w_i = 1 \quad (3.52)$$

$\rho(t)$  at time  $t$  is related to  $\rho(0)$  at time zero by this relation

$$\rho(t) = e^{-iHt} \rho(0) e^{iHt} \quad (3.53)$$

that is the time evaluation of density operator. If  $O$  is an operator, the expectation value of  $O$  is given by

$$\langle O \rangle = \text{Tr}(\rho O) \quad (3.54)$$

Because the trace is independent of representation,  $\text{Tr}(\rho O)$  can be evaluated by using any convenient basis. The relation in Eq.(3.54) is an extremely powerful relation to calculate the expectation value of any operator.

Density operator has two important properties. Firstly, it is Hermitian, as is evident from (3.1). Secondly, the density operator satisfies the normalisation condition

$$\text{Tr}(\rho) = 1 \quad (3.55)$$

and  $\rho$  follows equation of motion

$$\dot{\rho} = -\frac{i}{\hbar}(H\rho - \rho H) \quad (3.56)$$

In statistical mechanics, the probability  $w_n$  that the system is in the state described by an eigenket  $|\varphi_n\rangle$  is

$$w_n = \frac{e^{-\beta E_n}}{Z} \quad (3.57)$$

where  $\beta = \frac{1}{kT}$  and  $Z$  is the partition function which is defined by the equation

$$Z = \sum_n e^{-\beta E_n} = e^{-\beta F}, \quad F \equiv \text{free energy.} \quad (3.58)$$

Thus, the density matrix is

$$\rho = \sum_n \frac{e^{-\beta E_n}}{Z} |\varphi_n\rangle\langle\varphi_n| \quad (3.59)$$

In coordinate representation

$$\begin{aligned} \rho(x, x') &= \sum_n \frac{e^{-\beta E_n}}{Z} \varphi_n(x) \varphi_n^*(x') \\ &= \langle \varphi_n(x) \varphi_n^*(x') \rangle \end{aligned} \quad (3.60)$$

where  $\langle \rangle$  represents the average over the ensemble. One can see that this is the average of states which describe the systems in the ensemble. The trace of the density matrix is

$$\text{Tr}\rho(x, x') = \int dx dx' \delta(x - x') \rho(x, x') \quad (3.61)$$

and the expectation value of an operator  $O$  is

$$\langle O \rangle = \int dx dx' \rho(x, x') O(x, x'). \quad (3.62)$$

In the above

$$O(x, x') = \sum_{m, n} O_{mn} \varphi_m^*(x') \varphi_n(x) \quad (3.63)$$

and

$$O_{mn} = \int dx \varphi_m^*(x') O \varphi_n(x) \quad (3.64)$$

and  $\varphi_n(x)$  form a complete orthonormal set. For a density matrix  $\rho$  which is unnormalized Eq (3.60) replace to

$$\rho(x, x') = \sum_n e^{-\beta E_n} \varphi_n(x) \varphi_n^*(x') \quad (3.65)$$

This equation can lead us to formulate a path integral of density matrix by comparing with Feynman-Kac expansion of probability amplitude  $K(b, a)$ . The difference between the form of these two equations are in the argument of the exponential. If the time  $t_b - t_a$  in Eq.(3.15) is replaced by  $-i\hbar\beta$ , the result is the expression for the density matrix. Finally, we can (not discuss in detail) write the density matrix as the path integral

$$\rho(x, x') = \int_{x(\theta)}^{x(\hbar\beta)} Dx(u) \exp\left\{-\frac{i}{\hbar} \int_0^{\hbar\beta} du \left[\frac{m}{2}\dot{x}^2 + V(x)\right]\right\}. \quad (3.66)$$

This result gives the complete statistical behaviour of a quantum mechanical system as a path integral without the appearance  $i$  so characteristic of quantum mechanics. Notice that the variable  $u$  is not the real time in the usual sense (although it does have a dimension of time), it is just a parameter of density matrix. However, we can consider  $u$  as the time for a certain path  $x(u)$ , by which the system can go from initial point  $(x(\theta), \theta)$  to the final point  $(x(\hbar\beta), \hbar\beta)$ . The density matrix  $\rho(x, x')$  is a sum of contribution from each motion, the contribution from a particular motion being the exponential of the time integral of  $\frac{m}{2}\dot{x}^2 + V(x)$  divided by  $\hbar$  for the path in the equation. We see that if  $i$  in Eq (3.5) is replaced by  $u$  then we get Eq (3.66).

The partition function is

$$\begin{aligned} Z &= \int dx dx' \delta(x - x') \rho(x, x') \\ &= \int dx dx' Dx(u) \delta(x - x') \exp\left\{-\frac{i}{\hbar} \int_0^{\hbar\beta} du \left[\frac{m}{2}\dot{x}^2 + V(x)\right]\right\}. \end{aligned} \quad (3.67)$$

The formulation of density matrix  $\rho$  has the same form as the propagator  $K$ , so techniques to calculate the density matrix are also the same. Now we shall calculate a density matrix of a harmonic oscillator, say

$$\rho(x, x') = \int_{x(\theta)=x'}^{x(\hbar\beta)=x} Dx(u) \exp\left\{-\frac{i}{\hbar} \int_0^{\hbar\beta} du \left[\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2\right]\right\}. \quad (3.68)$$

Now  $A$  is defined as

$$A = \int_0^{\hbar\beta} du \left[\frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2\right] \quad (3.69)$$



$x_c(u)$  must satisfy the condition  $\delta A = 0$ , say

$$\delta A = - \int_0^{\hbar\beta} du [m\ddot{x} - m\omega^2 x] = 0$$

so that  $x_c(u)$  satisfies the equation

$$\ddot{x} - \omega^2 x = 0 \quad (3.70)$$

with boundary conditions

$$x(0) = x', \quad x(\hbar\beta) = x \quad (3.71)$$

hence

$$x_c(u) = \frac{1}{\sinh \omega\hbar\beta} [x \sinh \omega u + x' \sinh \omega(\hbar\beta - u)] \quad (3.72)$$

We find that

$$\begin{aligned} A_c &= A_c[x_c(u)] \\ &= \frac{m\omega}{2 \sinh \omega\hbar\beta} [(x^2 + x'^2) \cosh \omega\hbar\beta - 2xx'] \end{aligned} \quad (3.73)$$

and using (3.37),

$$F(\hbar\beta, 0) = \left( \frac{m\omega}{2\hbar\pi \sinh \omega\hbar\beta} \right)^{1/2} \quad (3.74)$$

So that the density matrix is

$$\rho(x, x') = \left( \frac{m\omega}{2\hbar\pi \sinh \omega\hbar\beta} \right)^{1/2} \exp \left\{ - \frac{m\omega}{2\hbar \sinh \omega\hbar\beta} [(x^2 + x'^2) \cosh \omega\hbar\beta - 2xx'] \right\} \quad (3.75)$$

Finally , we calculate the partition function as follows

$$Z = \int_{-\infty}^{\infty} dx \rho(x, x)$$

$$= \left( \frac{m\omega}{2\hbar\pi \sinh \omega\hbar\beta} \right)^{1/2} \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{m\omega(\cosh \omega\hbar\beta - 1)}{\hbar \sinh \omega\hbar\beta} x^2 \right\}$$

after integration we get the final result as

$$Z = \left( 2 \sinh \frac{\omega\hbar\beta}{2} \right)^{-1} \quad (3.76)$$

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