

Chapter 2

Feynman Path Integration

In this chapter Feynman path integration was presented. Unfortunately since the subject is large we cannot include all aspects. The interested readers are referred to [31, 32, 33, 34, 35]. In the first section we will explain the elements of path integral formulation and show that it is equivalent to the conventional formulation of Schrödinger and Heisenberg. Next we will give the examples that can be solved exactly. The third section is about statistical mechanics in the language of path integral. The final section is the variational method in terms of the propagator.

2.1 Path Integration in Nonrelativistic Quantum Mechanics

The standard formulation of quantum mechanics developed more or less concurrently by Schrödinger, Heisenberg and others in the 1920s, and shown to be equivalent to one another by Dirac. These approaches based on the Hamiltonian of the system which is a function of operators. In contrast Feynman path integral approach to quantum mechanics is tied to Lagrangian. Then no subtlety of commutability of operator is involved. The third formulation which developed in the 1940s by R. P. Feynman was inspired by P. A. M. Dirac's remarks [36, 37]. Dirac made the observation that the action plays a central role in classical mechanics, but seemed to have no important role in quantum mechanics as it was known at the time. He speculated on how this situation might be rectified,

and he arrived at the conclusion that the probability amplitude of a particle to arrive at particular space-time point “correspond to” $\exp\{iS/\hbar\}$, where S is the classical action evaluated along the classical path. Feynman further the idea by postulate that not just classical path contributes but all paths by the probability amplitude.

To get the picture of path integral let consider the double-slit experiment. Fig. 2.1 shows a diagram of double-slit experiment. The interference on the detecting screen arises from the superposition of two amplitude. Suppose we increase the number of slits from two to three. Then there will be three amplitude (see Fig. 2.2a) that we must add together to determine the probability amplitude that particle reaches a particular point on the detecting screen. Suppose we next insert another opaque screen with two slits behind the initial screen (Fig. 2.2b). Now there are six possible paths that the particle can takes to reach a point on the detecting screen. One can imagine filling up the space between the source and the detecting screen with an infinite series of opaque screens and then eliminating these screens with an infinite number of slits in each screen. In this way, we see that the probability amplitude for the particle to arrive at a point on the detecting screen with no barrier in between the source and the detector must be the sum of the amplitudes for the particle to take every path between the source and the detecting point. Then we are led to the following postulates:

- 1) All possible path contribute equally, i.e. formally in the same way as the amplitude; but different paths contribute with different phases.
- 2) The phase of the contribution of a given path is determined by the action S along this path (measured in \hbar).

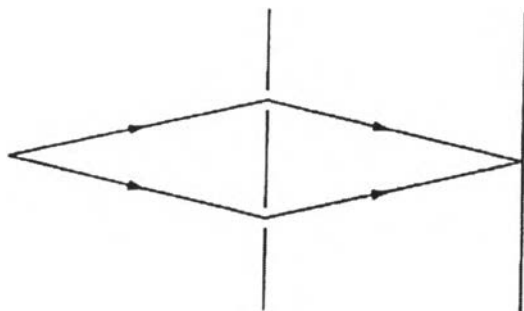
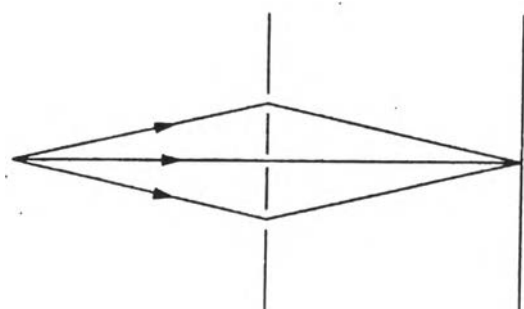
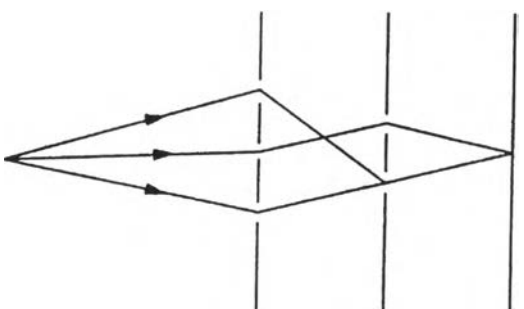


Figure 2.1: The two paths in the double-slit experiment. The amplitudes for these paths add together to produce an interference pattern on a distant detecting screen.



(a)



(b)

Figure 2.2: (a) The three paths for a triple-slit experiment. (b) Three of the six paths that a particle may follow to reach a particular point on the detecting screen when an additional screen with two slits is inserted.

The probability $P(b, a)$ that a particle will go from point x_a at time t_a to the point x_b at time t_b is defined by the absolute square of the complex amplitude $K(b, a)$, that is $P(b, a) = |K(b, a)|^2$. Furthermore the amplitude is given by a sum of contribution $\phi[x(t)]$ of all paths joining a and b , i.e.

$$K(b, a) = \sum_{\text{over all paths}} \phi[x(t)]. \quad (2.1)$$

The contribution of each path had a phase proportional to the action S along the path, i.e.

$$\phi[x(t)] = C \exp \{ (i/\hbar) \cdot S[x(t)] \}. \quad (2.2)$$

Here C is a normalization constant that has yet to be determined. It is the same for all paths, since all paths contribute with the same weight.

We will now discuss the sum contained in Eq. (2.2) in more detail and we will be guided by the analogy to Riemann's definition for an integral. For this we discretize the time interval $T = t_b - t_a$ into N equal partial intervals of length ϵ :

$$\left. \begin{array}{l} N\epsilon = t_b - t_a \\ \epsilon = t_{i+1} - t_i \\ t_0 = t_a \\ x_0 = x_a \end{array} \quad \begin{array}{l} t_b > t_a, \\ i = 1, \dots, N-1, \\ t_N = t_b, \\ x_N = x_b. \end{array} \right\} \quad (2.3)$$

Let x_a, t_a and x_b, t_b be the two fixed end points. We now construct a certain path by choosing special points x_i for all intermediate time points t_i and connect the selected points by straight line (see Fig. 2.3). By refining this lattice, we can approximate every path with any desired quality. Hence, it is natural to define the sum over all paths as a multiple integral over all values of x_i :

$$K(b, a) \sim \int dx_1 \cdots dx_{N-1} \phi[x(t)]. \quad (2.4)$$

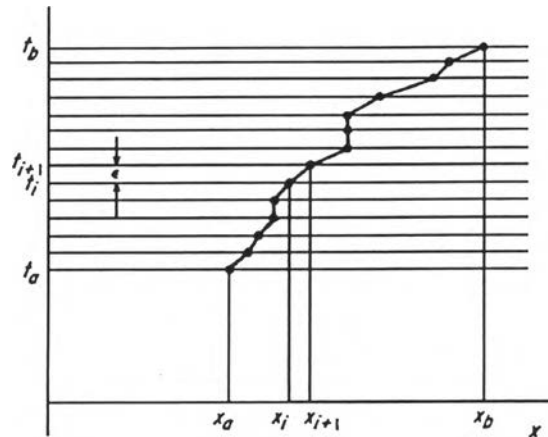


Figure 2.3: The sum over paths is defined as a limit, in which at first the path is specified by giving only its coordinate x at a large number of specified times separated by very small intervals ϵ . The path sum is then an integral over all these specific coordinates. Then to achieve the correct measure, the limit is taken as ϵ approaches 0.

Let us now define the sum implied in Eq. (2.1) more precisely. In Riemann's integral ϵ can be made smaller and smaller. Here one cannot directly operate a well-defined limiting value in this way. In order to force convergence, a normalization factor $A(\epsilon)$, depending on ϵ , has to be introduced. Summation lead to the path integral:

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \frac{dx_1}{A} \dots \frac{dx_{N-1}}{A} \exp \left\{ (i/\hbar) S[b, a] \right\}, \quad (2.5)$$

with the action define as

$$S[b, a] = \int_{t_a}^{t_b} dt L(x, \dot{x}, t). \quad (2.6)$$

S is the line integral along a route $dx_1 \dots dx_{N-1}$ through the points x_i . We write Eq. (2.5) in the abbreviation form:

$$K(b, a) = \int_a^b \mathcal{D}x(t) \exp \left\{ \frac{iS[b, a]}{\hbar} \right\} \quad (2.7)$$

where $\int_a^b \mathcal{D}x(t)$ denotes the infinite integral.

For the amplitude Eq. (2.5) and Eq. (2.7), an important property can be derived. Let consider the path integral for two successive events (see Fig. 2.4) with $t_a < t_c < t_b$. The action fulfills the obvious property:

$$S[b, a] = S[b, c] + S[c, a]. \quad (2.8)$$

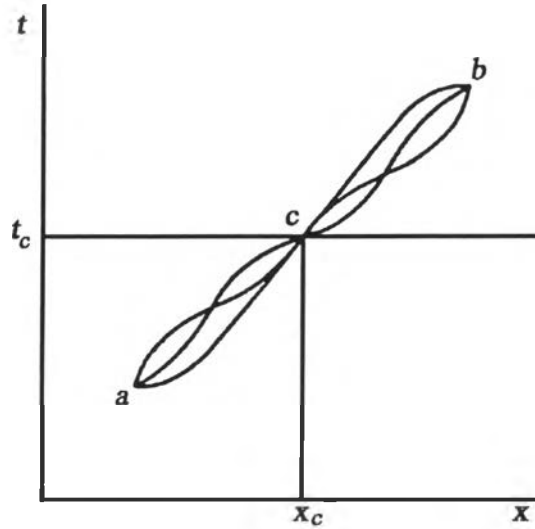


Figure 2.4: One way the sum over all paths can be taken is by first summing over paths which go through the point at x_c and time t_c . The amplitude on each path that goes from a to b via c is a product of two factors: (1) an amplitude to go from a to c and (2) an amplitude to go from c to b . This is therefore valid also for the sum over all paths through c : the total amplitude to go from a to b via c is $K(b, c)K(c, a)$. Thus summing over the alternatives (values of x_c), we get for the total amplitude to go from a to b , Eq. (2.11)

Now we consider Eq. (2.5)

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \frac{dx_1}{A} \dots \frac{dx_{M-1}}{A} \frac{dx_c}{A} \frac{dx_{M+1}}{A} \dots \frac{dx_{N-1}}{A} \times \exp \left\{ \frac{i}{\hbar} (S[b, c] + S[c, a]) \right\} \quad (2.9)$$

with $t_a < t_1 \dots < t_M < t_{M+1} \dots < t_b$.

The integration can be performed in any order, in particular as follow. First, for a fixed x_c , $S[c, a]$ a constant with respect to the integration over x_{M+1} up to

x_{N-1} . The same is valid for $S[b, c]$ with respect to the integrations over x_1 up to x_{M-1} . The integration over the point in between, x_c , is performed at the end.

Rewriting Eq. (2.9) accordingly yields

$$K(b, a) = \int dx_c \lim_{\epsilon \rightarrow 0} \left(\frac{1}{A} \int \frac{dx_1}{A} \cdots \frac{dx_{M-1}}{A} \exp \left\{ \frac{i}{\hbar} S[c, a] \right\} \right) \times \left(\frac{1}{A} \int \frac{dx_{M+1}}{A} \cdots \frac{dx_{N-1}}{A} \exp \left\{ \frac{i}{\hbar} S[b, c] \right\} \right), \quad (2.10)$$

which can also be denoted as

$$K(b, a) = \int dx_c K(b, c) K(c, a). \quad (2.11)$$

We can immediately generalize this to

$$K(b, a) = \int dx_1 \cdots dx_{N-1} K(b, N-1) K(N-1, N-2) \cdots \times \cdots K(i+1, i) \cdots K(1, a). \quad (2.12)$$

For an infinitesimal time interval $\epsilon = t_{i+1} - t_i$ between points x_{i+1} and x_i the following is valid up to first order in ϵ :

$$\begin{aligned} K(i+1, i) &= \frac{1}{A} \exp \left\{ \frac{i}{\hbar} S[i+1, i] \right\} \\ &= \frac{1}{A} \exp \left\{ \frac{i}{\hbar} \int_{t_i}^{t_{i+1}} dt L(x(t), \dot{x}(t), t) \right\} \\ &\approx \frac{1}{A} \exp \left\{ \frac{i\epsilon}{\hbar} L\left(\frac{x_{i+1} + x_i}{2}, \frac{x_{i+1} - x_i}{\epsilon}, \frac{\epsilon}{2}\right) \right\}. \end{aligned} \quad (2.13)$$

Thus the integral from Eq. (2.12), i.e. the amplitude for any complete path, can be written as

$$\phi[x(t)] = \lim_{\epsilon \rightarrow 0} \prod_{i=0}^{N-1} K(i+1, i). \quad (2.14)$$

For the case of a particle's motion in a potential $V(x)$ the Lagrangian, according to Eq. (2.13), read

$$L = \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 - V(x), \quad (2.15)$$

inserting into Eq. (2.12) yields

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int dx_1 \cdots dx_{N-1} \frac{1}{A^N} \exp \left[\frac{i\epsilon}{\hbar} \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 - V(x) \right]. \quad (2.16)$$

Now we want to prove that path integral approach is equivalent to the conventional approach. In the Feynman and Hibbs book [32], they use $K(b, a)$ to arrive at Schrödinger equation of motion. But we do this in reverse direction. Starting from Schrödinger equation we deduce path integral from it.

The Schrödinger of motion for time dependent state vector is

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) |\Psi(t)\rangle = 0. \quad (2.17)$$

Define Greens operator or time evolution operator by

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \hat{G}(t, t') = i\hbar \hat{1} \delta(t - t'). \quad (2.18)$$

In the x basis or spatial representation Eq. (2.18) becomes

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H}_x \right) G(x, t; x', t') = i\hbar \delta(x - x') \delta(t - t'), \quad (2.19)$$

where

$$G(x, t; x', t') = \langle x | \hat{G}(t, t') | x' \rangle. \quad (2.20)$$

Once \hat{G} is known, the time-dependent state $|\psi(t)\rangle$ can be deduced according to

$$|\Psi(t)\rangle = \hat{G}(t, t') |\Psi(t')\rangle. \quad (2.21)$$

For the case of a Hamiltonian \hat{H} that does not depend explicitly on time, a formal solution of Eq. (2.18) can be given immediately:

$$\hat{G}(t, t') = \theta(t - t') \exp \left(-\frac{i}{\hbar} \hat{H}(t - t') \right). \quad (2.22)$$

Here $\theta(t - t')$ is the Heaviside step function. The Greens function in space and time results from this as a matrix element

$$G(x, t; x', t') = \theta(t - t') \langle x | \exp\left(-\frac{i}{\hbar} \hat{H}(t - t')\right) | x' \rangle. \quad (2.23)$$

with $\hat{H} = \hat{T} + \hat{V}$. The following identity hold for the operator function:

$$\exp \hat{O} = \left[\exp(\hat{O}/N) \right]^N \quad (2.24)$$

If we substitute $\lambda = i(t - t')/\hbar$ into Eq. (2.23), the Greens function becomes

$$G(x, t; x', t') = \lim_{N \rightarrow \infty} \langle x | e^{-\lambda(\hat{T} + \hat{V})/N} e^{-\lambda(\hat{T} + \hat{V})/N} \dots e^{-\lambda(\hat{T} + \hat{V})/N} | x' \rangle, \quad (2.25)$$

with t always exceed t' .

We now apply the Trotter product (see Appendix A):

$$\lim_{N \rightarrow \infty} \left[\left(e^{-\lambda(\hat{T} + \hat{V})/N} \right)^N - \left(e^{-\lambda\hat{T}/N} e^{-\lambda\hat{V}/N} \right)^N \right] = 0, \quad (2.26)$$

and obtain

$$G(x, t; x', t') = \lim_{N \rightarrow \infty} \langle x | \left(e^{-\lambda\hat{T}/N} e^{-\lambda\hat{V}/N} \right)^N | x' \rangle. \quad (2.27)$$

Inserting a complete set of spatial states yield

$$G(x, t; x', t') = \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \prod_{i=0}^{N-1} \langle x_{i+1} | e^{-\lambda\hat{T}/N} e^{-\lambda\hat{V}/N} | x_i \rangle, \quad (2.28)$$

where $x_0 = x'$ and $x_N = x$. Now the matrix elements appearing in Eq. (2.28) have to be determined. Since the operator for the potential energy \hat{V} is diagonal in space, we have

$$\langle x_{i+1} | e^{-\lambda\hat{T}/N} e^{-\lambda\hat{V}/N} | x_i \rangle = \langle x_{i+1} | e^{-\lambda\hat{T}/N} | x_i \rangle e^{-\lambda V(x_i)/N}. \quad (2.29)$$

In order to calculate the spatial matrix element of the operator $e^{-\lambda\hat{T}/N}$ we insert a complete set of momentum eigenstates:

$$\begin{aligned}\langle x_{i+1}|e^{-\lambda\hat{T}/N}|x_i\rangle &= \int dp \langle x_{i+1}|e^{-\lambda\hat{T}/N}|p\rangle \langle p|x_i\rangle \\ &= \int dp \langle x_{i+1}|p\rangle \langle p|x_i\rangle e^{-\lambda p^2/2mN} \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp e^{-\lambda p^2/2mN} e^{ip(x_{i+1}-x_i)}.\end{aligned}\quad (2.30)$$

This is Gaussian integral in momentum space. We know that

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}.\quad (2.31)$$

Using this formulation we obtain

$$\langle x_{i+1}|e^{-\lambda\hat{T}/N}|x_i\rangle = \left(\frac{mN}{2\pi\lambda\hbar}\right)^{1/2} \exp\left[-\frac{mN(x_{i+1}-x_i)^2}{2\lambda\hbar^2}\right].\quad (2.32)$$

Inserting Eq. (2.32) and Eq. (2.29) into Eq. (2.28) result in

$$\begin{aligned}G(x, t; x', t') &= \lim_{N\rightarrow\infty} \int dx_1 \cdots dx_{N-1} \left(\frac{mN}{2\pi\lambda\hbar}\right)^{N/2} \\ &\quad \times \prod_{i=0}^{N-1} \exp\left[-\frac{mN}{2\lambda\hbar^2}(x_{i+1}-x_i)^2 - \frac{\lambda}{N}V(x_i)\right].\end{aligned}\quad (2.33)$$

We insert $\epsilon = (t-t')/N = \hbar\lambda/iN$ and sum the exponential expressions:

$$\begin{aligned}G(x, t; x', t') &= \lim_{\epsilon\rightarrow 0, N\rightarrow\infty} \int dx_1 \cdots dx_{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \\ &\quad \times \exp\left\{\frac{i\epsilon}{\hbar} \sum_{i=0}^{N-1} \left[\frac{m}{2}\left(\frac{x_{i+1}-x_i}{\epsilon}\right)^2 - V(x_i)\right]\right\}.\end{aligned}\quad (2.34)$$

This result is identical to the path integral in Eq. (2.16) and now the normalization constant is identified as

$$A(t) = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2}.\quad (2.35)$$

Note that Eq. (2.23) implied another property for the propagator

$$\lim_{t\rightarrow t'} G(x, t; x', t') = \delta(x-x').\quad (2.36)$$

2.2 Examples

We now calculate the free particle system as an example. The free particle is the system with $V = 0$. Then the propagator for the free particle is

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int dx_1 \cdots dx_{N-1} \frac{1}{A^N} \exp \left[\frac{im}{2\hbar\epsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2 \right], \quad (2.37)$$

with $x_0 = x_a, x_N = x_b$, and $N\epsilon = t_b - t_a$. The various integrations appearing in Eq. (2.37) are reducible to simple Gaussian integrals by means of the quadratic supplement in the exponent. The successive performance of the $N - 1$ integrations leads to a set of Gaussian integrations:

$$\int_{-\infty}^{\infty} dy e^{a(x-y)^2 + b(z-y)^2} = \left(\frac{-\pi}{a+b} \right)^{1/2} \exp \left[\frac{ab}{a+b} (x-z)^2 \right]. \quad (2.38)$$

Let us begin with the integration over x_1 ($\mu \equiv im/2\hbar\epsilon$):

$$\int_{-\infty}^{\infty} dx_1 e^{\mu(x_2-x_1)^2 + \mu(x_1-x_0)^2} = \left(\frac{-\pi}{2\mu} \right)^{1/2} e^{\mu(x_2-x_0)^2/2}. \quad (2.39)$$

Integration over x_2 gives:

$$\begin{aligned} \int_{-\infty}^{\infty} dx_2 \left(\frac{-\pi}{2\mu} \right)^{1/2} e^{\frac{\mu}{2}(x_2-x_0)^2 + \mu(x_3-x_2)^2} &= \left(\frac{-\pi}{2\mu} \right)^{1/2} \left(\frac{-\pi}{3\mu/2} \right)^{1/2} e^{\mu(x_3-x_0)^2/3} \\ &= \left(\frac{(-\pi)^2}{3\mu^2} \right)^{1/2} e^{\mu(x_3-x_0)^2/3}. \end{aligned} \quad (2.40)$$

Performance the $N - 1$ integration one after the other yields

$$\begin{aligned} \int_{-\infty}^{\infty} dx_1 \cdots dx_{N-1} e^{\{\mu[(x_N-x_{N-1})^2 + \dots + (x_1-x_0)^2]\}} \\ = \frac{1}{\sqrt{N}} \left(\frac{-\pi}{\mu} \right)^{(N-1)/2} e^{\mu(x_N-x_0)^2/2}. \end{aligned} \quad (2.41)$$

Then the propagator takes the form

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \frac{1}{A^N} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{N/2} \left(\frac{m}{2\pi i \hbar (t_b - t_a)} \right)^{1/2} \exp \left[\frac{im}{2\hbar} \frac{(x_b - x_a)^2}{(t_b - t_a)} \right]. \quad (2.42)$$

Putting Eq. (2.35) into Eq. (2.42) and take the limit $\epsilon \rightarrow 0$ we get

$$K(b, a) = \left(\frac{m}{2\pi i \hbar (t_b - t_a)} \right)^{1/2} \exp \left[\frac{im}{2\hbar} \frac{(x_b - x_a)^2}{(t_b - t_a)} \right]. \quad (2.43)$$

The next example is a harmonic oscillator system. But this time we shall not go through the tedious calculation as in case of the free particle, since we can determine the most important characteristics of the propagator in the following manner. Note that this technique apply to only a quadratic Lagrangian.

To illustrate how the method works, consider a particle whose Lagrangian has the form

$$L = a(t)\dot{x}^2 + b(t)x\dot{x} + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t). \quad (2.44)$$

Let $\bar{x}(t)$ be the classical path between the specific end points. This is the path which is an extremum for the action S . In the notation we have been using

$$S_{\text{cl}}[b, a] = S[\bar{x}(t)]. \quad (2.45)$$

Define the deviation of any path from \bar{x} as y (see Fig.2.5):

$$x = \bar{x} + y, \quad (2.46)$$

and the deviation y at the end points is zero

$$y(t_a) = y(t_b) = 0. \quad (2.47)$$

At each t the variables x and y differ by the constant \bar{x} . Therefore, clearly, $dx_i = dy_i$ for each specific point t_i in the subdivision of time. In general, we may say $\mathcal{D}x(t) = \mathcal{D}y(t)$.

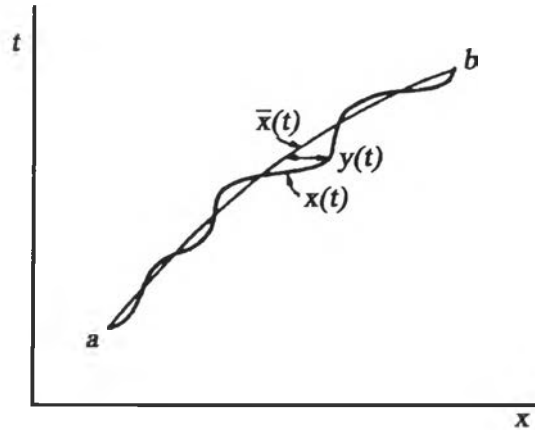


Figure 2.5: The difference between the classical path $\bar{x}(t)$ and some possible alternative path $x(t)$ is the function $y(t)$. Since the paths must both reach the same end points, $y(t_a) = y(t_b) = 0$. In between these end points $y(t)$ can take any form. Since the classical path is completely fixed, any variation in the alternative path $x(t)$ is equivalent to the associated variation in the difference $y(t)$. Thus, in a path integral, the path differential $\mathcal{D}x(t)$ can be replaced by $\mathcal{D}y(t)$, and the path $x(t)$ by $\bar{x}(t) + y(t)$. In this form \bar{x} is a constant for the integration over paths. Furthermore, the new path variable $y(t)$ is restricted to take the value 0 at both end points. This substitution leads to a path integral independent of end-point positions.

The integral for the action can be written

$$\begin{aligned} S[x(t)] &= S[\bar{x} + y(t)] \\ &= \int_{t_a}^{t_b} [a(t)(\dot{\bar{x}}^2 + 2\dot{\bar{x}}\dot{y} + \dot{y}^2) + \dots] dt. \end{aligned} \quad (2.48)$$

If all the terms which do not involve y are collected, the resulting integral is just $S[\bar{x}(t)] = S_{cl}$. If all the terms which contain y as a linear factor are collected, the resulting integral vanishes. The remaining terms are the second-order terms in y . Then

$$S[x(t)] = S_{cl}[b, a] + \int_{t_a}^{t_b} [a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2] dt. \quad (2.49)$$

The integral over paths does not depend upon the classical path, so the

propagator can be written

$$K(b, a) = e^{(i/\hbar)S_{cl}[b,a]} \int_0^0 \mathcal{D}y(t) \left(\exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} [a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2] dt \right\} \right). \quad (2.50)$$

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

$$K(b, a) = e^{(i/\hbar)S_{cl}[b,a]} F(t_b, t_a). \quad (2.51)$$

If the coefficients a, b and c are time-independent, then it follows that F is a function of the time difference: $F(t_b - t_a)$. Applying this technique to a harmonic oscillator which has a quadratic Lagrangian. Then the problem is to evaluate the classical action and prefactor $F(t_b - t_a)$.

It can be proved straightforwardly that the expression of the classical action is:

$$S_{cl}[b, a] = \frac{m\omega}{2 \sin(\omega T)} [(x_b^2 + x_a^2) \cos(\omega T) - 2x_a x_b], \quad (2.52)$$

where $T = t_b - t_a$ and $\omega T \neq n\pi$.

We employ the group property of $K(b, a)$, and Eq. (2.36). Thus

$$\begin{aligned} \delta(x_2 - x_1) &= K(x_2, t; x_1, t) \\ &= \int_{-\infty}^{\infty} dx K(x_2, t; x, 0) K(x, 0; x_1, t) \\ &= \int_{-\infty}^{\infty} dx K(x_2, t; x, 0) K^*(x_1, t; x, 0). \end{aligned} \quad (2.53)$$

Here we substitute

$$\left. \begin{aligned} K(x_2, t; x, 0) &= F(t) e^{(i/\hbar)S_{cl}(x_2, t; x, 0)} \\ K^*(x_1, t; x, 0) &= F^*(t) e^{-(i/\hbar)S_{cl}(x_1, t; x, 0)} \end{aligned} \right\}. \quad (2.54)$$

Hence we can continue to write

$$\delta(x_2 - x_1) = \int_{-\infty}^{\infty} dx |F(t)|^2 e^{(i/\hbar)[S_d(x_2, t; x, 0) - S_d(x_1, t; x, 0)]}. \quad (2.55)$$

The exponential can also be written as ($x_2 = x_1 + \Delta$);

$$\begin{aligned} S_d(x_1 + \Delta x, t; x, 0) - S_d(x_1, t; x, 0) &= \frac{\partial S_d(x_1, t; x, 0)}{\partial x_1} (x_2 - x_1) \\ &= \alpha(x)(x_2 - x_1), \end{aligned} \quad (2.56)$$

where

$$\begin{aligned} \alpha(x) &= \frac{\partial S_d(x_1, t; x, 0)}{\partial x_1} \\ &= \frac{\partial}{\partial x_1} \left(\frac{m\omega}{2 \sin(\omega t)} [(x_1^2 + x_2^2) \cos(\omega t) - 2x_1 x] \right) \\ &= \frac{m\omega}{\sin(\omega t)} (x_1 \cos(\omega t) - x). \end{aligned} \quad (2.57)$$

Note that $\alpha(x)$ is linear function of x , so that $\frac{dx}{d\alpha}$ is independence of x . With this information, we can continue to write

$$\begin{aligned} \delta(x_2 - x_1) &= \int_{-\infty}^{\infty} d\alpha \left| \frac{dx}{d\alpha} \right| |F(t)|^2 e^{(i/\hbar)\alpha(x)(x_2 - x_1)} \\ &= \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi\hbar} e^{(i/\hbar)\alpha(x)(x_2 - x_1)} \frac{2\pi\hbar |F(t)|^2}{|d\alpha/dx|}. \end{aligned} \quad (2.58)$$

From the definition of delta function

$$\delta(x_2 - x_1) = \int_{-\infty}^{\infty} e^{(i/\hbar)\alpha(x)(x_2 - x_1)} \frac{d\alpha}{2\pi\hbar},$$

then

$$|F(t)|^2 = \frac{1}{2\pi\hbar} \left| \frac{d\alpha}{dx} \right|. \quad (2.59)$$

From Eq. (2.57) we know that

$$\left| \frac{d\alpha}{dx} \right| = \frac{m\omega}{\sin(\omega t)}. \quad (2.60)$$

Finally we get

$$\begin{aligned} |F(t)|^2 &= \frac{m\omega}{2\pi\hbar\sin(\omega t)} \\ &= \frac{1}{2\pi\hbar} \frac{m}{t} \frac{1}{\sin(\omega t)/\omega t}. \end{aligned} \quad (2.61)$$

The phase of the prefactor $F(t)$ can be determined from our knowledge of the free particle propagator. Using $\lim_{x \rightarrow 0} \frac{\sin x}{x} = 1$, we obtain from Eq. (2.43)

$$F(t) \longrightarrow \sqrt{\frac{m}{2\pi i \hbar t}} \quad \text{for } \omega \rightarrow 0 \quad (2.62)$$

Thereby we have found the propagator for the linear harmonic oscillator ($T = t_b - t_a$):

$$K(x_b, t_b; x_a, t_a) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \exp\left(\frac{i m \omega}{2 \hbar \sin(\omega T)} [(x_b^2 + x_a^2) \cos(\omega T) - 2x_b x_a]\right). \quad (2.63)$$

2.3 Statistical Mechanics via Path Integral

The path integral turns out to provide an elegant way of doing statistical mechanics. And since Bose-Einstein condensation is the result of quantum statistical mechanics, we then want to describe how path integral connect to statistical mechanics.

The prime quantity in statistical mechanics is the partition function which express in the form below:

$$Z = \sum_{j=0}^{\infty} e^{-\beta E_j}, \quad (2.64)$$

where $\beta = 1/k_B T$ and T is temperature in the absolute unit. E_j is the energy of the state $|j\rangle$. We can rewrite this as

$$\mathcal{Z} = \text{Tr} e^{-\beta H}, \quad (2.65)$$

where the trace is taken in the eigenbasis of H

$$H|j\rangle = E_j|j\rangle. \quad (2.66)$$

Now we exploit the fact that the trace is invariant under a unitary change of basis and switch to the x -basis to obtain

$$\mathcal{Z} = \int_{-\infty}^{\infty} \langle x|e^{-\beta H}|x\rangle dx. \quad (2.67)$$

Then the integrand is defined as density matrix:

$$\rho(x, x') = \langle x|e^{-\beta H}|x'\rangle, \quad (2.68)$$

inserting the complete set of energy eigenstates obtain:

$$\begin{aligned} \rho(x, x') &= \sum_j \langle x|e^{-\beta H}|j\rangle \langle j|x'\rangle \\ &= \sum_j \phi_j(x') \phi_j^*(x) e^{-\beta E_j}, \end{aligned} \quad (2.69)$$

where $\phi_j(x')$ means the eigenfunction corresponds to the eigenstate j .

Recall that the propagator is a time translation matrix element Eq. (2.23)

$$\begin{aligned} K(x, t; x', t') &= \langle x|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle \\ &= \sum_j \langle x|e^{-\frac{i}{\hbar}H(t-t')}|j\rangle \langle j|x'\rangle \\ &= \sum_j \phi_j(x') \phi_j^*(x) e^{-\frac{i}{\hbar}E_j(t-t')}. \end{aligned} \quad (2.70)$$

It is easily seen that the density matrix bears a close resemblance to the propagator. The only difference between them is lied in the argument of the exponential term. Actually if we set $(t - t')$ equal to $-i\beta\hbar$ the Eq. (2.70) is identical to Eq. (2.69). In other word, the density matrix is the propagator in the negative imaginary time. In ordinary (real) time,

$$K(x, T; x', 0) = \int \mathcal{D}x(t) \exp \left\{ \frac{i}{\hbar} \int_0^T dt \left(\frac{m\dot{x}^2}{2} - V(x) \right) \right\}. \quad (2.71)$$

With $T \rightarrow -i\beta\hbar$,

$$K(x, -i\beta\hbar; x', 0) = \int \mathcal{D}x(t) \exp \left\{ \frac{i}{\hbar} \int_0^{-i\beta\hbar} dt \left(\frac{m\dot{x}^2}{2} - V(x) \right) \right\} \quad (2.72)$$

where we now integrate along the negative imaginary time axis (Figure 2.6).

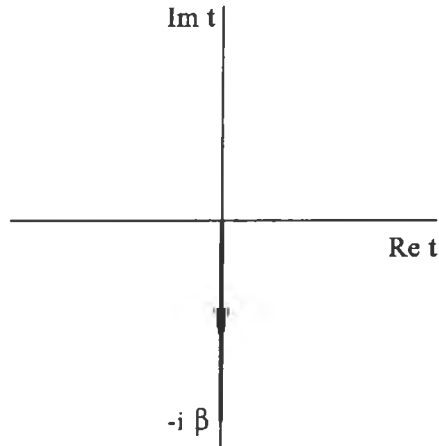


Figure 2.6: Path in the complex time plane.

Let us define a real variable for this integration, $\tau = it$. τ is called the imaginary time, since when the time t is imaginary, τ is real. Then integral over τ is along its real axis: when $t = 0 \rightarrow -i\beta\hbar$, then $\tau = 0 \rightarrow \beta\hbar$. We can write x as a function of the variable τ : $x(t) \rightarrow x(\tau)$; then $\dot{x} = i \frac{dx}{d\tau}$. The propagator

becomes

$$\begin{aligned} K(x, -i\beta\hbar; x', 0) &= \int \mathcal{D}x(\tau) \exp \left\{ \frac{-1}{\hbar} \int_0^{\beta\hbar} \left(\frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right) d\tau \right\} \\ &= \int \mathcal{D}x(\tau) \exp \left\{ \frac{-1}{\hbar} \int_0^{\beta\hbar} \mathcal{L}_E(x, \dot{x}) d\tau \right\}. \end{aligned} \quad (2.73)$$

\mathcal{L}_E is called the euclidean Lagrangian. Note that \mathcal{L}_E is the sum of the euclidean kinetic energy and real time potential energy. Thus the particle obeying the euclidean equations of motion will see the potential upside down.

2.4 Variational Method

There are very few system which can be solved exactly either in Hamiltonian or Lagrangian approach. Then some approximations are needed. Hence in this section we shall now describe perturbation technique for the evaluation of the path integral defining the partition, applicable to those system where S is real.

Suppose we wish to evaluate the free energy of a system. The problem can be expressed in terms of path integrals by starting with the partition function defined as

$$\mathcal{Z} = e^{-\beta F}. \quad (2.74)$$

In Eq. (2.67) it was expressed as an integral over the density matrix. In Eq. (2.73) the density matrix is expressed in terms of path integral. Then it allows us to write

$$\mathcal{Z} = \int \int_{x_1}^{x_1} \exp \left\{ -\frac{S}{\hbar} \right\} \mathcal{D}x(\tau) dx_1 \quad (2.75)$$

where

$$S = \int_0^{\beta\hbar} \mathcal{L}_E(x, \dot{x}) d\tau.$$

From now on we are choosing units in such a way that the value of \hbar is 1. It can be so included by a straightforward dimension inspection.

Suppose that some other S' can be found which satisfies two conditions: First, S' is simple enough that expression such as $\int e^{-S'} \mathcal{D}x(\tau)$ or $\int G e^{-S'} \mathcal{D}x(\tau)$, for simple functionals G , can be evaluated. Second, the important paths in the integral $\int e^{-S} \mathcal{D}x(\tau)$ and those in the integral $\int e^{-S'} \mathcal{D}x(\tau)$ are similar, that is, S' and S are similar when they are both small. And let F' be the free energy associated with S' . Then

$$e^{-\beta(F-F')} = \frac{\int \int_{x_1}^{x_1} e^{-S} \mathcal{D}x(\tau) dx_1}{\int \int_{x_1}^{x_1} e^{-S'} \mathcal{D}x(\tau) dx_1}. \quad (2.76)$$

Then since $e^{-S} = e^{-(S-S')} e^{-S'}$, we write Eq. (2.76) as

$$\begin{aligned} e^{-\beta(F-F')} &= \frac{\int \int_{x_1}^{x_1} e^{-(S-S')} e^{-S'} \mathcal{D}x(\tau) dx_1}{\int \int_{x_1}^{x_1} e^{-S'} \mathcal{D}x(\tau) dx_1} \\ &= \langle e^{-(S-S')} \rangle_{S'}, \end{aligned} \quad (2.77)$$

where the subscript S' means that the weighting function is the path integral corresponds to S' . This means that $e^{-\beta(F-F')}$ is the average value of $e^{-(S-S')}$ where this average is take over all paths with the same initial and final point and the weight of each path is $e^{-S'} \mathcal{D}x(\tau)$.

Introducing Feynman-Jensen inequality which states that the average of x when x is a random variable always exceeds or equals the exponential of the average value of x , as long as x is real and the weights used in the averaging process are positive. That is,

$$\langle e^{-x} \rangle \geq e^{-\langle x \rangle}, \quad (2.78)$$

where $\langle x \rangle$ = the weighted average of x . The geometrical interpretation of this relation is as shown in Fig. 2.7.

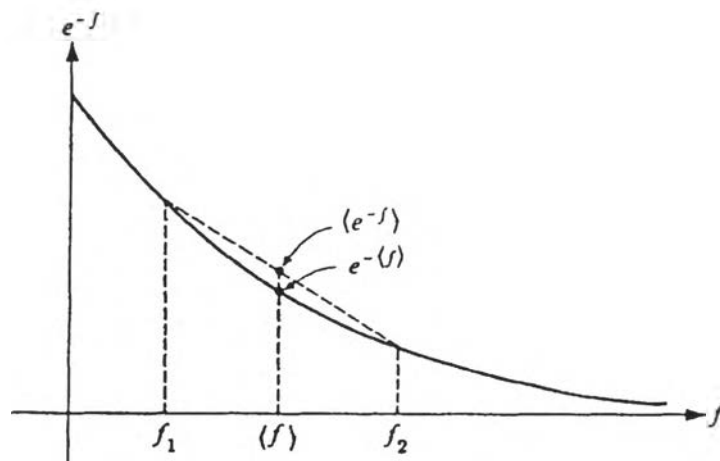


Figure 2.7: Geometrical interpretation of $\langle e^{-f} \rangle \geq e^{-\langle f \rangle}$

Now Eq. (2.77) becomes

$$\begin{aligned} e^{-\beta(F-F')} &= \langle e^{-(S-S')} \rangle_{S'} \\ &\geq e^{-\langle S-S' \rangle_{S'}}. \end{aligned} \quad (2.79)$$

This result implies that

$$F \leq F' + \delta, \quad (2.80)$$

where

$$\delta = \frac{1}{\beta} \langle S - S' \rangle_{S'}.$$

This is a minimum principle which says that, if we calculate $F' + \delta$ for various “actions” S' , that calculation which gives the smallest result is nearest to the true free energy. Or if only a reasonable general form of S' can be guessed but certain parameters still remain uncertain, the calculation of $F' + \delta$ can be made leaving

these parameters undetermined. Then the nearest approximation of F will be the lowest $F' + \delta$ available. That is, the “best” values of the parameters are those which minimize $F' + \delta$.

This principle can be used to find an approximation value for the lowest energy state of the system E_0 . Recall that

$$\mathcal{Z} = e^{-\beta F} = \sum_{j=0}^{\infty} e^{-\beta E_j}. \quad (2.81)$$

As the temperature becomes lower and lower, this is, as β grows larger, the contribution of each state decreases exponentially. At the limit $\beta \rightarrow \infty$ the ground state dominates the rest in the series. That is

$$\lim_{\beta \rightarrow \infty} \mathcal{Z} = e^{-\beta E_0}. \quad (2.82)$$

This means that at large β we can replace F by E_0 . Then Eq. (2.80) becomes

$$E_0 \leq E'_0 + \delta. \quad (2.83)$$

In approximating E_0 we can disregard the specification that the initial and final points of the paths be the same. To understand this, we refer back to Eq. (2.69) and note that as β becomes large the density matrix $\rho(x', x)$ is also dominated by the zero-order term and approach $e^{-\beta E_0} \phi_0(x') \phi_0^*(x)$. Thus the dependence on x and x' enter into a multiplying factor but does not affect the nature of the exponential behavior of the function. It is this exponential behavior which is fundamental in the evaluation of E_0 by this technique.