CHAPTER 2

Path Integral Formulation

2.1 Show by direct substitution that the free particle kernel $K(x_f, t; x_i, 0)$ satisfies the differential equation $\mathrm{i}\hbar\partial K/\partial t = -(\hbar^2/2m)\partial^2 K/\partial x_f^2$.

From

$$K(x_f, t; x_i, 0) = \left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{1/2} \mathrm{e}^{\mathrm{i}m(x_f - x_i)^2/(2\hbar t)}$$

we obtain

$$\begin{aligned}
\frac{\partial K}{\partial t} &= -\frac{K}{2t} - \frac{\mathrm{i}m}{2\hbar}\left(\frac{x_f - x_i}{t}\right)^2 K\,, \\
\frac{\partial K}{\partial x_f} &= \frac{\mathrm{i}m}{\hbar}\frac{(x_f - x_i)}{t} K
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial^2 K}{\partial x_f^2} &= \frac{\mathrm{i}mK}{\hbar t} + \mathrm{i}m\frac{(x_f - x_i)}{t}\frac{\partial K}{\partial x_f} \\
&= \frac{\mathrm{i}mK}{\hbar t} + \left(\frac{\mathrm{i}m}{\hbar}\right)^2 \left(\frac{x_f - x_i}{t}\right)^2 K \\
&= -\frac{2m}{\hbar^2}\left[-\mathrm{i}\hbar\frac{K}{2t} + \frac{m}{2}\left(\frac{x_f - x_i}{t}\right)^2 K\right] \\
&= -\frac{2m}{\hbar^2}\left(\mathrm{i}\hbar\frac{\partial K}{\partial t}\right)\,.
\end{aligned}$$

That is,

$$\mathrm{i}\hbar\frac{\partial K}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 K}{\partial x_f^2}\,.$$

2.2 Find the wavelength λ of oscillation of $K(x,t;0,0)$ of a free particle at large values of x at a fixed time.

We have

$$K(x,t;0,0) = \left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{1/2} \mathrm{e}^{\mathrm{i}mx^2/(2\hbar t)} \ .$$

The phase factor is given by $mx^2/(2\hbar t)$. Increasing x by λ must increase the phase of K by 2π. That is,

$$\begin{aligned} 2\pi &= \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t} \\ &= \frac{mx\lambda}{\hbar t} + \frac{m\lambda^2}{2\hbar t} \ . \end{aligned}$$

For large values of x, $\dfrac{m\lambda^2}{2\hbar t} \ll \dfrac{mx\lambda}{\hbar t}$. Therefore,

$$2\pi \approx \frac{mx\lambda}{\hbar t} \quad \text{or} \quad \lambda = \frac{2\pi\hbar}{mx/t} \ .$$

Since mx/t is the classical momentum p, we get $\lambda = h/p$.

2.3 Show that for a fixed distance x, the frequency of oscillation of $K(x,t;0,0)$ at large values of t is given by $\nu = E/h$ where E is the classical energy of the free particle.

If T is the period of oscillation then changing $t \to t+T$ will change the phase factor $mx^2/(2\hbar t)$ by 2π. Hence,

$$2\pi = \frac{mx^2}{2\hbar t} - \frac{mx^2}{2\hbar(t+T)} = \frac{mx^2 T}{2\hbar t^2(1+\frac{T}{t})} \ .$$

For large values of t, we get $2\pi \approx mx^2T/(2\hbar t^2)$. That is,

$$\frac{1}{T} = \frac{1}{2\pi\hbar}\frac{mx^2}{2t^2} \ .$$

Since $v = x/t$ and $mx^2/(2t^2) = E$ we obtain $1/T = \nu = E/h$.

2.4 Obtain the classical action for one-dimensional harmonic oscillator.

The Lagrangian for one-dimensional harmonic oscillator is

$$L = \frac{m}{2}\left(\dot{x}^2 - \omega^2 x^2\right) \ . \tag{2.1}$$

Substituting $\dot{x}^2 = \dfrac{\mathrm{d}}{\mathrm{d}t}(x\dot{x}) - x\ddot{x}$ in the above equation we get

$$L = \frac{m}{2}\left(\frac{\mathrm{d}}{\mathrm{d}t}(x\dot{x}) - x\ddot{x} - \omega^2 x^2\right) \ . \tag{2.2}$$

Since the equation of motion for a linear harmonic oscillator is $m\ddot{x} + \omega^2 x = 0$ we get $L = \frac{m}{2}\frac{\mathrm{d}}{\mathrm{d}t}x\dot{x}$. Then

$$S(x_{\mathrm{CM}}(t)) = \int_{t_i=0}^{t_f=T} L\mathrm{d}t = \frac{m}{2}\left[(x\dot{x})_{t=T} - (x\dot{x})_{t=0}\right] \ . \tag{2.3}$$

Using the solution $x(t) = A\cos\omega t + B\sin\omega t$ of the linear harmonic oscillator with $A = x(0) = x_i$ and $B\omega = \dot{x}(0) = \dot{x}_i$ we get

$$x_f = x(T) = x_i\cos\omega T + \frac{\dot{x}_i}{\omega}\sin\omega T \ , \tag{2.4}$$

$$\dot{x}_f = \dot{x}(T) = \omega x_i \sin\omega T + \dot{x}_i\cos\omega T \ . \tag{2.5}$$

From Eq. (2.4) we get

$$\dot{x}_i = \frac{(x_f - x_i\cos\omega T)\omega}{\sin\omega T} \tag{2.6}$$

Using this expression in Eq. (2.5) we obtain

$$\dot{x}_f = \frac{(-x_i + x_f\cos\omega T)\omega}{\sin\omega T} \ . \tag{2.7}$$

Using (2.6) and (2.7) we get

$$x_f\dot{x}_f - x_i\dot{x}_i = \frac{\omega\left[(x_i^2 + x_f^2)\cos\omega T - 2x_i x_f\right]}{\sin\omega T} \tag{2.8}$$

and

$$S(x_{\mathrm{CM}}(t)) = \frac{m\omega}{2\sin\omega T}\left[(x_i^2 + x_f^2)\cos\omega T - 2x_i x_f\right] \ . \tag{2.9}$$

2.5 Express the propagator in terms of eigenstates.

In the operator formalism the time-independent Schrödinger equation is

$$H|\phi_n\rangle = E_n|\phi_n\rangle \ ,$$

where

$$\langle\phi_m|\phi_n\rangle = \delta_{mn} \ , \quad \sum_n |\phi_n\rangle\langle\phi_n| = 1 \ .$$

In the coordinate basis

$$|\phi_n\rangle = \int \mathrm{d}x\, \phi_n(x)|x\rangle \ , \quad \phi_n(x) = \langle x|\phi_n\rangle$$

and

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi_n}{\mathrm{d}x^2}+V\phi_n=E_n\phi_n\ .$$

Then

$$|\psi(t)\rangle=\sum_n C_n\mathrm{e}^{-\mathrm{i}E_nt/\hbar}|\phi_n\rangle$$

or

$$\psi(x,t)=\sum_n C_n\mathrm{e}^{-\mathrm{i}E_nt/\hbar}\phi_n(x)\ .$$

Now, we write

$$\begin{aligned}K(x_f,T;x_i,0) &= \langle x_f|\mathrm{e}^{-\mathrm{i}HT/\hbar}|x_i\rangle\\ &= \langle x_f|\mathrm{e}^{-\mathrm{i}HT/\hbar}\sum|\phi_n\rangle\langle\phi_n|x_i\rangle\\ &= \sum\langle x_f|\phi_n\rangle\mathrm{e}^{-\mathrm{i}E_nT/\hbar}\langle\phi_n|x_i\rangle\\ &= \sum_n\psi_n(x_f)\psi_n^*(x_i)\mathrm{e}^{-\mathrm{i}E_nT/\hbar}\ .\end{aligned}$$

2.6 Similar to the quantum statistical function $Z(\beta)=\mathrm{Tr}\,\mathrm{e}^{-\beta H}$ we can introduce the quantum mechanical partition function as $Z(t_f,t_i)=\mathrm{Tr}\,U(t_f,t_i)$. Obtain the path integral form of it.

In the time-independent case

$$Z(t_f,t_i)=Z(t_f-t_i)=\mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}(t_f-t_i)H/\hbar}\ .$$

$Z(\beta)$ and $Z(t_f,t_i)$ are related by continuation of t_f-t_i as $t_f-t_i=-\mathrm{i}\hbar\beta$. Computing the trace in $|n\rangle$ basis we get

$$Z(t_f-t_i)=\sum_n\mathrm{e}^{-\mathrm{i}(t_f-t_i)E_n/\hbar}\tag{2.1}$$

In $|x\rangle$ basis

$$\begin{aligned}Z(t_f-t_i) &= \int_{-\infty}^{\infty}\mathrm{d}x\langle x|U(t_f,t_i)|x\rangle\\ &= \int_{-\infty}^{\infty}K(x,x;t_f-t_i)\mathrm{d}x.\end{aligned}$$

$x_f=x_i=x$ means that the integration is over all closed paths at x.

Then

$$\begin{aligned} Z(t_f,t_i) &= N\int_{-\infty}^{\infty}\mathrm{d}x\int_{x(t_i)=x}^{x(t_f)=x}\mathcal{D}[x(t)]\,\mathrm{e}^{\mathrm{i}S[x(t)]/\hbar} \\ &= N\int_{x(t_f)=x(t_i)}\mathcal{D}[x(t)]\,\mathrm{e}^{\mathrm{i}S[x(t)]/\hbar} \\ &= \int_{x(t_f)=x(t_i)}\hat{\mathcal{D}}[x(t)]\,\mathrm{e}^{\mathrm{i}S[x(t)]/\hbar}\,. \end{aligned} \tag{2.2}$$

Comparing (2.2) with (2.1) we infer that by computing this path integral over all closed loops we can determine the energy eigenvalues.

2.7 Obtain the propagator for a particle of mass m confined within a box potential $V(x) = 0$ for $|x| < a$ and ∞ for $|x| > a$.

By solving the Schrödinger equation of the given problem we obtain

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}, \quad \psi_n(x) = \sqrt{\frac{2}{a}}\sin(n\pi x/a)\ .$$

The propagator is then obtained as

$$K(x_f,t;x,0) = \frac{2}{a}\sum_{j=1}^{\infty}\exp\left[-\frac{\mathrm{i}\hbar\pi^2 j^2}{2ma^2}\right]\sin(j\pi x_f/a)\sin(j\pi x_i/a)\ .$$

We need to include all paths joining the initial point x_i and the end point x_f within a period of time t. There are infinite paths connecting x_i and x_f because the walls of the potential reflects the particles incident on it. Four of these paths are shown in Fig. 7. *Do these all paths distinct?*

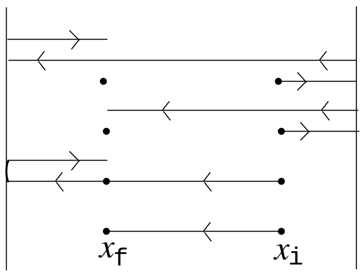

FIGURE 2.1 Some of the paths connecting x_i and x_f for a particle in a box potential system.

No. Instead of considering particles reflected at the walls we remove the walls and set-up a sequence of mirror reflected boxes on either sides of the original box. We view the particle as a free particle. In this case

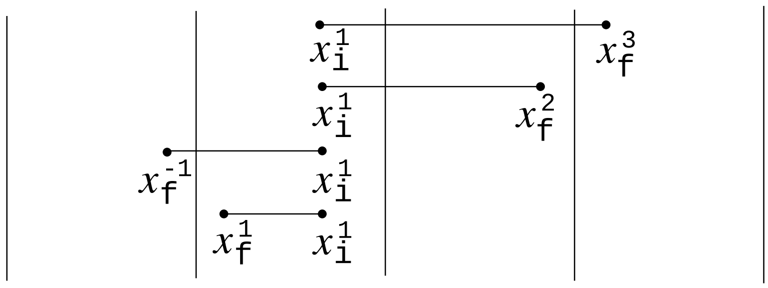

FIGURE 2.2 Paths corresponding to those in Fig. 2.1 when instead of reflecting the particle at the wall it is allowed to pass through the sequence of mirror reflected boxes.

there will not be folding of paths. The paths in Fig.7 become those in Fig. 7. From this figure we observe that for an odd number of reflections the end point is at $2na - x_f$ while for even number of reflections the end point becomes $2na + x_f$. Therefore, we have

$$\begin{aligned} K_{\text{odd}}^{(2n-1)}(x_f, t; x_i, 0) &= \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \exp\left[\frac{\mathrm{i}m}{2\hbar t}(2na - x_f - x_i)^2\right] \\ K_{\text{even}}^{(2n)}(x_f, t; x_i, 0) &= \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \exp\left[\frac{\mathrm{i}m}{2\hbar t}(2na + x_f - x_i)^2\right] . \end{aligned}$$

Remember that we need to consider only the paths that are not crossing the walls. We can write the resultant propagator as the propagator that includes all the paths minus the propagator that considers only the paths which crossed the walls. By a tricky argument (for details see G.L. Ingold, Path integrals and their applications to dissipative quantum systems (preprint)) we obtain

$$K(x_f, t; x_i, 0) = K_{\text{even}}^{(2n)} - K_{\text{odd}}^{(2n+1)} .$$

2.8 Making use of the propagator of a free particle the propagator for a particle of mass confined to a ring of radius R.

The stationary state eigenfunctions and energy eigenvalues of the system obtained by solving the Schrödinger equation is

$$\psi_l(\phi) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}l\phi}, \quad E_l = \frac{\hbar^2 l^2}{2mR^2}, \quad l = 0, \pm 1, \pm 2, \cdots .$$

The propagator for a free particle is

$$K(x_f, t; x_i, 0) = \left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{1/2} \mathrm{e}^{\mathrm{i}m(x_f - x_i)^2/2\hbar t} .$$

There is a difference between free particle and a particle on a ring. In the ring case we need to find the angles $\phi + 2\pi n$, where n is an integer and ϕ is the angle. There are infinite number of paths connecting ϕ_i and ϕ_f. These paths are different. For example one path is connecting ϕ_i and ϕ_f without making one complete revolution over the ring. Another path is starting from ϕ_i crossing ϕ_f and then ϕ_i and then ending on ϕ_f (that is, connecting after making one revolution). In this case the winding number is 1. In this way different paths are characterized by winding number. Two paths with distinct winding number cannot be continuously transformed into one another. Thus all paths can be taken into consideration by summing over all winding numbers. That is, the propagator consists of sum of all free particle's propagators with various winding numbers. This gives (G.L. Ingold, Path integrals and their applications to dissipative quantum systems (preprint))

$$K(\phi_f, t; \phi_i, 0) = R\left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{1/2} \sum \exp\left[\frac{\mathrm{i}mR^2}{2\hbar t}(\phi_f - \phi_i - 2\pi n)^2\right] .$$

In the above the presence R is because the coordinate of the particle on a ring is specified by an angle rather than a position.

Because the propagator is periodic with period-2π in $\phi_f - \phi_i$ we write

$$K(\phi_f, t; \phi_i, 0) = \sum_{l=-\infty}^{\infty} C_l \mathrm{e}^{\mathrm{i}l(\phi_f - \phi_i)} ,$$

where

$$C_l = \frac{1}{2\pi} \mathrm{e}^{-\mathrm{i}\hbar l^2 t/(2mR^2)} .$$