Path Intergal

Shoichi Midorikawa

1 Introduction

The Feynman path integral[1] is one of the formalism to solve the Schrödinger equation. However this approach is not peculiar to quantum mechanics, and M. Kac[2] is the one who recognized the applicability to the diffusion equation. Therefore, this formula is nowadays known as Feynman-Kac formula.

The purpose of this note is to derive the path integral from the Schrödinger equation in a general way so that it can also be applicable to the diffusion equation. I will also show a somewhat different way to calculate the prefactor of the kernel of the simple harmonic oscillator.

2 Derivation From Schrödinger Equation

Consider the one-dimensional Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t). \tag{1}$$

The formal solution is

$$\psi(x,t) = \exp\left[-\frac{i}{\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)t\right]\psi(x,0).$$

We can rewrite

$$\psi(x,t) = \int_{-\infty}^{\infty}\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)t\right]\delta(x-x_0)\psi(x_0,0)\,dx_0$$

The kernel is defined by

$$K(x,t;x_0,t_0) = \exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)(t-t_0)\right]\delta(x-x_0) \tag{2}$$

Then we have

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t;x_0,t_0)\psi(x_0,t_0)\,dx_0 \tag{3}$$

The successive use of eq.(3) leads to

$$\begin{aligned}\psi(x_c,t_c) &= \int_{-\infty}^{\infty} K(x_c,t_c;x_b,t_b)\psi(x_b,t_b)\,dx_b \\ &= \int_{-\infty}^{\infty} K(x_c,t_c;x_b,t_b)\{K(x_b,t_b;x_a,t_a)\rho(x_a,t_a)\,dx_a\}\,dx_b\end{aligned}$$

This leads to the following relationship between the kernels

$$K(x_c,t_c;x_a,t_a) = \int_{-\infty}^{\infty} K(x_c,t_c;x_b,t_b)K(x_b,t_b;x_a,t_a)\,dx_b$$

Let

$$\begin{aligned}&N\epsilon = t \\ &\epsilon = t_{i+1} - t_i \ (i = 0,1,2,\cdots,t_N) \\ &t_0 = 0, \quad t_N = t \\ &x_0 = 0, \quad x_N = x\end{aligned}$$

and

$$K(i+1;i) = K(x_{i+1},t_{i+1};x_i,t_i)$$

for abbreviation. Then,

$$\begin{aligned}K(x,t;0,0) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} K(N;N-1)K(N-1;N-2) \\ &\qquad \cdots K(2;1)K(1;0)\,dx_{N-1}\cdots dx_2\,dx_1\end{aligned} \tag{4}$$

Furthermore, we have for small ϵ

$$\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\epsilon\right] =$$

$$\exp\left[-\frac{i}{\hbar}V(x)\epsilon\right]\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\epsilon\right] - \frac{\epsilon^2}{2\hbar^2}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}, V(x)\right] + \mathcal{O}(\epsilon^3)$$

Thus

$$\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\epsilon\right] \to \exp\left[-\frac{i}{\hbar}V(x)\epsilon\right]\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\epsilon\right]$$

as $\epsilon \to 0$.

Using the integral representation of the delta function

$$\delta(x_i - x_{i-1}) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x_i-x_{i-1})/\hbar}\,dp$$

we can evaluate $K(i;i-1)$ in the limit of $\epsilon \to 0$:

$$\begin{aligned}
K(i;i-1) &= \frac{1}{2\pi\hbar}e^{-\frac{i}{\hbar}V(x_i)\epsilon}\int_{-\infty}^{\infty} dp\,\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\epsilon\right]e^{ip(x_i-x_{i-1})/\hbar} \\
&= \frac{1}{2\pi\hbar}e^{-\frac{i}{\hbar}V(x_i)\epsilon}\int_{-\infty}^{\infty} dp\,\exp\left[-\frac{i}{\hbar}\left(\frac{p^2}{2m}\epsilon - p(x_i-x_{i-1})\right)\right] \\
&= \frac{1}{2\pi\hbar}e^{-\frac{i}{\hbar}V(x_i)\epsilon}\int_{-\infty}^{\infty} dp\,\exp\left[-\frac{i\epsilon}{2m\hbar}\left(p-\frac{m(x_i-x_{i-1})}{\epsilon}\right)^2\right. \\
&\qquad\qquad\left.+i\frac{m(x_i-x_{i-1})^2}{2\epsilon\hbar}\right]
\end{aligned}$$

The p integral is of the Gaussian form

$$\int_{-\infty}^{\infty} e^{-\frac{p^2}{2\sigma^2}}\,dp = \sqrt{2\pi\sigma^2}$$

We will apply this formula even in case of imaginary σ^2. Substitution of $\sigma^2 = \frac{m\hbar}{i\epsilon}$ gives

$$K(i;i-1) = \sqrt{\frac{m}{2\pi i\hbar\epsilon}}\exp\left\{\frac{i}{h}\epsilon\left[\frac{m}{2}\left(\frac{x_i-x_{i-1}}{\epsilon}\right)^2 - V(x_i)\right]\right\} \qquad (5)$$

By substituiting eq.(5) into eq.(4) and taking the limit of $\epsilon \to 0$, we obtain

$$\begin{aligned}
K(x,t;0,0) &= \lim_{\epsilon\to 0}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int\cdots\int dx_1\cdots dx_{N-1} \\
&\quad\times\exp\left\{\frac{i}{h}\epsilon\sum_{i=1}^{N}\left[\frac{m}{2}\left(\frac{x_i-x_{i-1}}{\epsilon}\right)^2 - V(x_i)\right]\right\} \qquad (6)
\end{aligned}$$

In a continuum limit

$$\epsilon \sum_{i=1}^{N} \left[\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\epsilon} \right)^2 - V(x_i) \right]$$
$$\Rightarrow \int_0^t dt \, \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) = \int_0^t dt \, L(\dot{x}, x) = S\left(x(t)\right)$$

where $L(\dot{x}, x)$ is a Langrangian and $S\left(x(t)\right)$ is the action. Furthermore we define the notation

$$\int \mathfrak{D}x(t) = \lim_{\epsilon \to 0} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{N/2} \int \cdots \int dx_1 \cdots dx_{N-1}$$

Then we have

$$K(x, t; 0, 0) = \int \mathfrak{D}x(t) \exp\left[\frac{i}{\hbar} S(x(t)) \right]$$

3 Harmonic Oscillator

The Lagrangian of the harmonic oscillator is

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

We wish to calculate

$$K[b; a] = \int_a^b \mathfrak{D}x(t) \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} dt \, L\left(\dot{x}(t), x(t)\right) \right]$$

the integral over all paths which go from (x_a, t_a) to (x_b, t_b).

We can represent x in terms of classical path x_c and quantum fluctuation y around classical path;

$$x(t) = x_c(t) + y(t) \qquad \text{with} \qquad y(t_b) = y(t_a) = 0$$

Then,

$$\begin{aligned} \frac{m}{2} \left(\dot{x}^2 - \omega^2 x^2 \right) &= \frac{m}{2} \left\{ (\dot{x}_c + \dot{y})^2 - \omega^2 (x_c + y)^2 \right\} \\ &= \frac{m}{2} \left(\dot{x}_c^2 - \omega^2 x_c^2 \right) + m(\dot{x}_c \dot{y} - \omega^2 x_c y) + \frac{m}{2} \left(\dot{y}^2 - \omega^2 y^2 \right) \end{aligned}$$

The action is

$$S[b,a] = \int_{t_a}^{t_b} \frac{m}{2}\left(\dot{x}_c^2 - \omega^2 x_c^2\right)\,dt - \int_{t_a}^{t_b} m(\dot{x}_c\dot{y} - \omega^2 x_c y)\,dt + \int_{t_a}^{t_b} \frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\,dt$$

The second term is, using integration by parts,

$$\int_{t_a}^{t_b} m(\dot{x}_c\dot{y} - \omega^2 x_c y)\,dt = m\dot{x}_c y|_{t_a}^{t_b} - \int_{t_a}^{t_b} m(\ddot{x}_c + \omega^2 x_c)y\,dt$$

which vanishes because $y(t_a) = y(t_b) = 0$ and $\ddot{x}_c + \omega^2 x_c = 0$. Thus $S[b,a]$ can be divided into two parts. the classcal and the quantum parts;

$$S[b,a] = S_{cl}[b,a] + S_q[0,0]$$

Notice that $S_q[0,0]$ is a function of the time interval $T = t_b - t_a$. This means that $K(b;a)$ must be of the form

$$K(b;a) = F(T)e^{\frac{i}{\hbar}S_{cl}[b,a]}$$

where

$$F(T) = \int_0^0 \exp\left[\frac{i}{\hbar}\int_0^T \frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\,dt\right]\mathfrak{D}y(t) \tag{7}$$

Now we evaluate $S_{cl}[b,a]$. We write

$$y(t) = A\cos(\omega t + \varphi_a).$$

Then $x_a = A\cos\varphi_a,\ x_b = A\cos(\omega T + \varphi_a)$, where $T = t_b - t_a$. The classical action represented by x_a and x_b is

$$S_{cl}[b,a] \quad = \quad \frac{m\omega}{2}\Big(-x_a x_b \sin\omega T - A\sin\varphi_a\left(x_b\cos\omega T - x_a\right)\Big) \tag{8}$$

Since $x_b = A\cos(\omega T + \varphi_a) = x_a\cos\omega T - A\sin\varphi_a\sin\omega T$,
we have

$$A\sin\varphi_a = \frac{x_a\cos\omega T - x_b}{\sin\omega T}$$

By substituting this into eq.(8), we have

$$\begin{aligned} S_{cl}[b,a] &= \frac{m\omega}{2}\left(-x_a x_b \sin\omega T - \frac{(x_b\cos\omega T - x_a)(x_a\cos\omega T - x_b)}{\sin\omega T}\right) \\ &= \frac{m\omega}{2\sin\omega T}\left((x_a^2+x_b^2)\cos\omega T - 2x_a x_b\right) \end{aligned}$$

Determination Of The Prefactor

We evaluate

$$F(T) = \int_0^0 \exp\left[\frac{i}{\hbar}\int_0^T \frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\, dt\right]\mathfrak{D}y(t) \tag{9}$$

by discritizing the functional integral $\mathfrak{D}y(t)$, namely,

$$= \lim_{\epsilon\to 0}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int_0^0 \exp\left[-\frac{m}{2i\epsilon}\sum_{i=1}^{N}\left((y_i - y_{i-1})^2 - \omega^2\epsilon^2 y_i^2\right)\right] dy_1 dy_2\cdots dy_{N-1}$$

Note that $y_0 = y_N = 0$. We express the sum in the exponent in terms of the vector and matrix notation

$$\sum_{i=1}^{N}\left((y_i - y_{i-1})^2 - \omega^2\epsilon^2 y_i^2\right) = \boldsymbol{y}^T M_{N-1}\boldsymbol{y}$$

where

$$\boldsymbol{y}^T = (y_1,\ y_2,\ \cdots\cdots\ ,\ y_{N-2},\ y_{N-1})$$

and

$$M_{N-1} = \begin{pmatrix} 2-\omega^2\epsilon^2 & -1 & 0 & \cdots\cdots & 0 & 0 & 0 \\ -1 & 2-\omega^2\epsilon^2 & -1 & \cdots\cdots & 0 & 0 & 0 \\ 0 & -1 & 2-\omega^2\epsilon^2 & \cdots\cdots & 0 & 0 & 0 \\ & \vdots & & \ddots & & \vdots & \\ 0 & 0 & 0 & \cdots\cdots & 2-\omega^2\epsilon^2 & -1 & 0 \\ 0 & 0 & 0 & \cdots\cdots & -1 & 2-\omega^2\epsilon^2 & -1 \\ 0 & 0 & 0 & \cdots\cdots & 0 & -1 & 2-\omega^2\epsilon^2 \end{pmatrix}$$

The recursive formula of $\det M_n$ is

$$\det M_n = (2-\omega^2\epsilon^2)\det M_{n-1} - \det M_{n-2},$$

and the characteric equation is

$$x^2 - (2-\omega^2\epsilon^2)x + 1 = 0$$

The solution of this equation is

$$x = \left(1 - \frac{\omega^2\epsilon^2}{2}\right) \pm i\omega\epsilon\sqrt{1-\frac{\omega^2\epsilon^2}{4}} \equiv \cos\theta \pm i\sin\theta$$

Note that,

$$\begin{aligned}
\det M_1 &= 2-\omega^2\epsilon^2 = 2\cos\theta = \frac{\sin 2\theta}{\sin\theta} \\
\det M_2 &= (2-\omega^2\epsilon^2)^2 - 2(2-\omega^2\epsilon^2) = \frac{\sin 3\theta}{\sin\theta} \\
\det M_3 &= 2\cos\theta\cdot\frac{\sin 3\theta}{\sin\theta} - \frac{\sin 2\theta}{\sin\theta} = \frac{\sin 4\theta}{\sin\theta}
\end{aligned}$$

We can show

$$\det M_{N-1} = \frac{\sin N\theta}{\sin\theta}$$

by mathematical induction. Hece,

$$\begin{aligned}
F(T) &= \lim_{\epsilon\to 0}\sqrt{\frac{m}{2\pi i\epsilon}\frac{1}{\det M_{N-1}}} = \lim_{\epsilon\to 0}\sqrt{\frac{m}{2\pi i\epsilon}\frac{\sin\theta}{\sin N\theta}} \\
&= \sqrt{\frac{m\omega}{2\pi i\sin T\omega}}
\end{aligned}$$

where we have used

$$T = N\epsilon, \quad \lim_{\epsilon\to 0}\sin\theta = \lim_{\epsilon\to 0}\theta = \omega\epsilon, \quad \text{and} \quad \lim_{\epsilon\to 0}\sin N\theta = \sin N\omega\epsilon = \sin T\omega.$$

Finally the kernel for the harmonic oscillator is

$$K(b;a) = \sqrt{\frac{m\omega}{2\pi i\sin T\omega}}\exp\left\{\frac{i}{\hbar}\left[\frac{m\omega}{2\sin\omega T}\left((x_a^2+x_b^2)\cos\omega T - 2x_ax_b\right)\right]\right\}$$

References

[1] R. Feynman, Space-Time Approach to Non-Relativistic Quantum Mechanics (1948) Rev. Modern Physics. 20.
R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path Integrals (McGrawHill, New York, 1965).

[2] M.Kac, Transactions of the American Mathematical Society 65(1949)1-13.