Introduction To The Path Intergal

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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   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

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

Then we have

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

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

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

and

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

for abbreviation. Then,

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

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

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

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 $\epsilon \to 0$:

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

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 $\sigma^2 = \dfrac{m\hbar}{i\epsilon}$ 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

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

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,

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

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

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

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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

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

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

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

$$= \frac{m\omega}{2\sin\omega T}\left(\left(x_a^2 + x_b^2\right)\cos\omega T - 2x_a x_b\right)$$

Determination of $F(T)$

We evaluate

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

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 $y_0 = y_N = 0$ and

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

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where

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

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 soution of this equation is given by

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

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 proof that

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

by mathematical induction. Hece,

$$F(T) = \lim_{\epsilon\to 0} \sqrt{\frac{m}{2\pi i\epsilon}\frac{\sin\theta}{\sin N\theta}} = \sqrt{\frac{m\omega}{2\pi i\sin T\omega}}$$

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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 given by

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

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.