

# Path Integral

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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 Derivation From Schrödinger Equation

Consider the one-dimensional Schrödinger equation

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

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

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

and

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

for abbreviation. Then,

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

Furthermore, we have for small  $\epsilon$

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

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  $\epsilon \rightarrow 0$ .

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  $\epsilon \rightarrow 0$ :

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

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  $\sigma^2$ . Substitution of  $\sigma^2 = \frac{m\hbar}{i\epsilon}$  gives

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

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

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

In a continuum limit

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

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

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

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

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

We wish to calculate

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

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;

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

Then,

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

The action is

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

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

$$F(T) = \int_0^1 \exp \left[ \frac{i}{\hbar} \int_0^T \frac{m}{2} (\dot{y}^2 - \omega^2 y^2) dt \right] \mathfrak{D}y(t) \quad (7)$$

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

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

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

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

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

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

Note that  $y_0 = y_N = 0$  and

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

where

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

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 show that

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

by mathematical induction. Hece,

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

where we have used

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

Finally the kernel for the harmonic oscillator is

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

## 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.