

# Chapter 2: Path Integral Formalism of Quantum Mechanics

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## 1 Definition of Propagator

### Time Independent Case

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle \quad (1)$$

$H$  不含时, 波函数可以写成 ( $t'$  是  $t$  之前的任意一个时间点)

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar} H(t-t')\right] |\psi(t')\rangle \quad (2)$$

将  $\langle \vec{r} |$  作用在方程两边

$$\langle \vec{r} | \psi(t) \rangle = \langle \vec{r} | \exp\left[-\frac{i}{\hbar} H(t-t')\right] |\psi(t')\rangle \quad (3)$$

单位算符  $\int d\vec{r}' |\vec{r}'\rangle \langle \vec{r}'| = 1$  作用在方程右边

$$\langle \vec{r} | \psi(t) \rangle = \int d\vec{r}' \langle \vec{r} | \exp\left[-\frac{i}{\hbar} H(t-t')\right] |\vec{r}'\rangle \langle \vec{r}' | \psi(t') \rangle \quad (4)$$

$$\psi(\vec{r}, t) = \langle \vec{r} | \psi(t) \rangle \quad (5)$$

$$\psi(\vec{r}, t) = \int d\vec{r}' \langle \vec{r} | \exp\left[-\frac{i}{\hbar} H(t-t')\right] |\vec{r}'\rangle \psi(\vec{r}', t') = \int d\vec{r}' K(\vec{r}, t; \vec{r}', t') \psi(\vec{r}', t') \quad (6)$$

在物理上,  $K(\vec{r}, t; \vec{r}', t')$  被称为传播子 (propagator), 在数学上是 Kernel 或 Green's function。定义

$$K(\vec{r}, t; \vec{r}', t') = \langle \vec{r} | \exp\left[-\frac{i}{\hbar} H(t-t')\right] |\vec{r}'\rangle \quad (7)$$

当  $t = t'$  时

$$K(\vec{r}, t; \vec{r}', t') = \langle \vec{r} | \vec{r}' \rangle = \delta(\vec{r} - \vec{r}') \quad (8)$$

假定  $H$  存在一系列本征态和相应的本征值

$$H |n\rangle = E_n |n\rangle \quad (9)$$

$|n\rangle$  构成完备基, 存在单位算符

$$|n\rangle \langle n| = 1 \quad (10)$$

$$\begin{aligned}
K(\vec{r}, t; \vec{r}', t') &= \langle \vec{r} | \exp \left[ -\frac{i}{\hbar} H(t - t') \right] | \vec{r}' \rangle \\
&= \sum_n \sum_{n'} \langle \vec{r} | n \rangle \langle n | \exp \left[ -\frac{i}{\hbar} H(t - t') \right] | n' \rangle \langle n' | \vec{r}' \rangle \\
&= \sum_n \sum_{n'} \psi_n(\vec{r}) \delta_{n,n'} \psi_{n'}^\dagger(\vec{r}') \exp \left[ -\frac{i}{\hbar} E_n(t - t') \right] \\
&= \sum_n \psi_n(\vec{r}) \psi_n^\dagger(\vec{r}') e^{-\frac{i}{\hbar} E_n(t - t')} \\
&= \sum_n \left[ \psi_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t} \right] \left[ \psi_n(\vec{r}') e^{-\frac{i}{\hbar} E_n t'} \right]^\dagger \\
&= \sum_n \psi_n(\vec{r}, t) \psi_n^\dagger(\vec{r}', t')
\end{aligned} \tag{11}$$

### Example: The Free Particle

$$H = -\frac{\hbar^2}{2m} \nabla^2 \tag{12}$$

自由粒子的解是平面波

$$\psi_{\vec{p}}(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \exp \left[ \frac{i}{\hbar} \left( \vec{p} \cdot \vec{r} - \frac{p^2}{2m} t \right) \right] \tag{13}$$

其传播子

$$\begin{aligned}
K(\vec{r}, t; \vec{r}', t') &= \int \psi_{\vec{p}}(\vec{r}, t) \psi_{\vec{p}}^\dagger(\vec{r}', t') d\vec{p} \\
&= \frac{1}{(2\pi\hbar)^3} \int d\vec{p} \exp \left[ \frac{i\vec{p}}{\hbar} (\vec{r} - \vec{r}') - \frac{ip^2}{2m\hbar} (t - t') \right]
\end{aligned} \tag{14}$$

由于

$$d\vec{p} = dp_x dp_y dp_z \tag{15}$$

且  $dp_x, dp_y, dp_z$  等价

$$\begin{aligned}
&\int_{-\infty}^{\infty} dp_x \exp \left[ \frac{i}{\hbar} p_x (x - x') - \frac{i}{2m\hbar} p_x^2 (t - t') \right] \\
&= \int_{-\infty}^{\infty} dp_x \exp \left\{ \left[ -\frac{i}{2m\hbar} (t - t') \right] \left( p_x^2 - 2mp_x \frac{x - x'}{t - t'} \right) \right\} \\
&= \int_{-\infty}^{\infty} dp_x \exp \left\{ \left[ -\frac{i}{2m\hbar} (t - t') \right] \left[ \left( p_x - m \frac{x - x'}{t - t'} \right)^2 - m^2 \frac{(x - x')^2}{(t - t')^2} \right] \right\} \\
&= \exp \left[ \frac{im(x - x')^2}{2\hbar(t - t')} \right] \int_{-\infty}^{\infty} dp_x \exp \left\{ \left[ -\frac{i}{2m\hbar} (t - t') \right] \left[ \left( p_x - m \frac{x - x'}{t - t'} \right)^2 \right] \right\} \\
&= \exp \left[ \frac{im(x - x')^2}{2\hbar(t - t')} \right] \int_{-\infty}^{\infty} dp_x \exp \left[ -\frac{i}{2m\hbar} (t - t') p_x^2 \right]
\end{aligned} \tag{16}$$

根据 Euler integral

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \tag{17}$$

$$\int_{-\infty}^{\infty} dp_x \exp \left[ \frac{i}{\hbar} p_x (x - x') - \frac{i}{2m\hbar} p_x^2 (t - t') \right] = \exp \left[ \frac{im(x - x')^2}{2\hbar(t - t')} \right] \sqrt{\frac{2m\pi\hbar}{i(t - t')}} \tag{18}$$

故

$$K(\vec{r}, t; \vec{r}', t') = \left[ \frac{2\pi i \hbar}{i(t-t')} \right]^{\frac{3}{2}} \exp \left[ \frac{im(\vec{r} - \vec{r}')^2}{2\hbar(t-t')} \right] \quad (19)$$

General Case

回到前面不含时情况下的波函数

$$\begin{aligned} \psi(\vec{r}, t) &= \int d\vec{r}' \langle \vec{r} | \exp \left[ -\frac{i}{\hbar} H(t-t') \right] | \vec{r}' \rangle \psi(\vec{r}', t') \\ &= \int d\vec{r}' \langle \vec{r} | \exp \left[ -\frac{i}{\hbar} H(t-t''+t''-t') \right] | \vec{r}' \rangle \psi(\vec{r}', t') \\ &= \int d\vec{r}' \langle \vec{r} | \exp \left[ -\frac{i}{\hbar} H(t-t'') \right] \exp \left[ -\frac{i}{\hbar} H(t''-t') \right] | \vec{r}' \rangle \psi(\vec{r}', t') \\ &= \int d\vec{r}' \int d\vec{r}'' \langle \vec{r} | \exp \left[ -\frac{i}{\hbar} H(t-t'') \right] | \vec{r}'' \rangle \langle \vec{r}'' | \exp \left[ -\frac{i}{\hbar} H(t''-t') \right] | \vec{r}' \rangle \psi(\vec{r}', t') \\ &= \int d\vec{r}' \int d\vec{r}'' K(\vec{r}, t; \vec{r}'', t'') K(\vec{r}'', t''; \vec{r}', t') \psi(\vec{r}', t') \end{aligned} \quad (20)$$

又

$$\psi(\vec{r}, t) = \int d\vec{r}' K(\vec{r}, t; \vec{r}', t') \psi(\vec{r}', t') \quad (21)$$

即

$$K(\vec{r}, t; \vec{r}', t') = \int d\vec{r}'' K(\vec{r}, t; \vec{r}'', t'') K(\vec{r}'', t''; \vec{r}', t') \quad (22)$$

因此

$$K(\vec{r}, t; \vec{r}', t') = \int d\vec{r}_1 \int d\vec{r}_2 \cdots \int d\vec{r}_{N-1} K(\vec{r}, t; \vec{r}_{N-1}, t_{N-1}) K(\vec{r}_{N-1}, t_{N-1}; \vec{r}_{N-2}, t_{N-2}) \cdots K(\vec{r}_1, t_1; \vec{r}', t') \quad (23)$$

## 2 Equation of Motion for $K(\vec{r}, t; \vec{r}', t')$

前面我们讨论的都是比较熟悉的薛定谔方程里面的东西，接下来我们来研究  $K(\vec{r}, t; \vec{r}', t')$  的另一个性质，即讨论格林函数  $K(\vec{r}, t; \vec{r}', t')$  的运动方程。

$$\psi(\vec{r}, t) = \int K(\vec{r}, t; \vec{r}', t') \psi(\vec{r}', t') d\vec{r}' \quad (24)$$

将  $(i\hbar \frac{\partial}{\partial t} - H)$  算符作用在方程两边

$$0 = \int \left[ \left( i\hbar \frac{\partial}{\partial t} - H \right) K(\vec{r}, t; \vec{r}', t') \right] \psi(\vec{r}', t') d\vec{r}' \quad (25)$$

因此我们得到  $K$  的运动方程

$$\left( i\hbar \frac{\partial}{\partial t} - H \right) K(\vec{r}, t; \vec{r}', t') = 0 \quad (26)$$

传播子代表是  $t'$  时刻对  $t$  时刻的影响，也就是说  $t$  时刻的性质是由  $t'$  时刻决定的，且  $t > t'$ 。当  $t < t'$  时，若  $K \neq 0$ ，则代表后面时刻  $t'$  可以影响前面时刻  $t$ ，这显然是不对的。因此

$$\begin{cases} (i\hbar \frac{\partial}{\partial t} - H) K(\vec{r}, t; \vec{r}', t') = 0 & (t > t') \\ K(\vec{r}, t; \vec{r}', t') = 0 & (t < t') \end{cases} \quad (27)$$

在  $t = t'$  时, 有奇性 (singular), 即

$$\left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') = c(\vec{r}, \vec{r}') \delta(t - t') \quad (28)$$

接下来我们来确定  $c(\vec{r}, \vec{r}')$ , 两边积分

$$\int_{-\infty}^{\infty} \left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') dt = \int_{-\infty}^{\infty} c(\vec{r}, \vec{r}') \delta(t - t') dt \quad (29)$$

$$\begin{aligned} \text{LHS} &= \int_{-\infty}^{t'-} \left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') dt + \int_{t'-}^{t'+} \left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') dt \\ &\quad + \int_{t'+}^{\infty} \left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') dt \\ &= \int_{t'-}^{t'+} \left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') dt = \int_{t'-}^{t'+} i\hbar \frac{\partial}{\partial t} K(\vec{r}, t; \vec{r}', t') dt \\ &= i\hbar K(\vec{r}, t = t'; \vec{r}', t') \end{aligned} \quad (30)$$

当  $H$  不含时时,  $K(\vec{r}, t = t'; \vec{r}', t') = \delta(\vec{r} - \vec{r}')$ , 因此

$$\text{LHS} = i\hbar \delta(\vec{r} - \vec{r}') \quad (31)$$

$$\text{RHS} = \int_{-\infty}^{\infty} c(\vec{r}, \vec{r}') \delta(t - t') dt = c(\vec{r}, \vec{r}') \quad (32)$$

由 LHS=RHS 得

$$c(\vec{r}, \vec{r}') = i\hbar \delta(\vec{r} - \vec{r}') \quad (33)$$

则

$$\left(i\hbar \frac{\partial}{\partial t} - H\right) K(\vec{r}, t; \vec{r}', t') = i\hbar \delta(\vec{r} - \vec{r}') \delta(t - t') \quad (34)$$

这就是  $K(\vec{r}, t; \vec{r}', t')$  的运动方程。

### 3 Time-dependent Case

前面我们讨论的都是  $H$  不含时的情况, 接下来我们讨论  $H$  含时的情况

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (35)$$

可以将波函数写成以下形式

$$|\psi(t)\rangle = U(t, t') |\psi(t')\rangle \quad (36)$$

$U(t, t')$  为演化算符 (evolution operator), 将  $|\psi(t)\rangle$  代回薛定谔方程得到

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H(t) U(t, t') \quad (37)$$

对波函数作用  $\langle \vec{r} |$

$$\langle \vec{r} | \psi(t) \rangle = \langle \vec{r} | U(t, t') | \psi(t') \rangle = \int d\vec{r}' \langle \vec{r} | U(t, t') | \vec{r}' \rangle \langle \vec{r}' | \psi(t') \rangle \quad (38)$$

即

$$\psi(\vec{r}, t) = \int d\vec{r}' K(\vec{r}, t; \vec{r}', t') \psi(\vec{r}', t') \quad (39)$$

定义普遍情况的传播子

$$K(\vec{r}, t; \vec{r}', t') = \langle \vec{r} | U(t, t') | \vec{r}' \rangle \quad (40)$$

不断重复作用演化算符，可以得到

$$U(t, t') = U(t, t_{N-1})U(t_{N-1}, t_{N-2}) \cdots U(t_1, t') \quad (41)$$

因此

$$\begin{aligned} K(\vec{r}, t; \vec{r}', t') &= \langle \vec{r} | U(t, t') | \vec{r}' \rangle = \langle \vec{r} | U(t, t_{N-1})U(t_{N-1}, t_{N-2}) \cdots U(t_1, t') | \vec{r}' \rangle \\ &= \int d\vec{r}_{N-1} \int d\vec{r}_{N-2} \cdots \int d\vec{r}_1 \langle \vec{r} | U(t, t_{N-1}) | \vec{r}_{N-1} \rangle \langle \vec{r}_{N-1} | U(t_{N-1}, t_{N-2}) | \vec{r}_{N-2} \rangle \cdots \langle \vec{r}_1 | U(t_1, t') | \vec{r}' \rangle \\ &= \int d\vec{r}_{N-1} \int d\vec{r}_{N-2} \cdots \int d\vec{r}_1 K(\vec{r}, t; \vec{r}_{N-1}, t_{N-1}) K(\vec{r}_{N-1}, t_{N-1}; \vec{r}_{N-2}, t_{N-2}) \cdots K(\vec{r}_1, t_1; \vec{r}', t') \end{aligned} \quad (42)$$

很容易发现并验证

$$U^\dagger(t, t') = U(t, t') \quad (43)$$

$$-i\hbar \frac{\partial}{\partial t} U^\dagger(t, t') = H(t)U^\dagger(t, t') \quad (44)$$

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(t') | U^\dagger(t, t') U(t, t') | \psi(t') \rangle = 1 \quad (45)$$

因此

$$U^\dagger(t, t') U(t, t') = 1 \quad (46)$$

$$U^\dagger(t, t') = U^{-1}(t, t') = U(t, t') \quad (47)$$

因此  $U$  是么正算符 (unitary operator)

定义

$$|\vec{r}, t\rangle = U^\dagger(t, 0) |\vec{r}\rangle \quad (48)$$

则

$$\langle \vec{r}, t | = \langle \vec{r} | U(t, 0) \quad (49)$$

$$\begin{aligned} K(\vec{r}, t; \vec{r}', t') &= \langle \vec{r} | U(t, t') | \vec{r}' \rangle = \langle \vec{r} | U(t, 0) U(0, t') | \vec{r}' \rangle \\ &= \langle \vec{r} | U(t, 0) U^\dagger(0, t') | \vec{r}' \rangle = \langle \vec{r}, t | \vec{r}', t' \rangle \end{aligned} \quad (50)$$

接下来讨论特殊情况：H(t)=H

$$U(t, t') = \exp\left[-\frac{iH(t-t')}{\hbar}\right] \quad (51)$$

$$U(t, 0) = \exp\left(-\frac{iHt}{\hbar}\right) \quad (52)$$

$$\begin{aligned} |\vec{r}, t\rangle &= U^\dagger(t, 0) |\vec{r}\rangle = \exp\left(\frac{iHt}{\hbar}\right) |\vec{r}\rangle = \sum_n \exp\left(\frac{iHt}{\hbar}\right) |n\rangle \langle n | \vec{r} \rangle \\ &= \sum_n \exp\left(\frac{iHt}{\hbar}\right) |n\rangle \psi_n^\dagger(\vec{r}) = \sum_n |n\rangle \exp\left(\frac{iE_n t}{\hbar}\right) \psi_n^\dagger(\vec{r}) \end{aligned} \quad (53)$$

$$\begin{aligned} K(\vec{r}, t; \vec{r}', t') &= \langle \vec{r}, t | \vec{r}', t' \rangle = \sum_n \sum_m \langle m | \exp\left(-\frac{iE_m t}{\hbar}\right) \psi_m(\vec{r}) \exp\left(\frac{iE_n t'}{\hbar}\right) \psi_n^\dagger(\vec{r}') | n \rangle \\ &= \sum_n \exp\left[\frac{iE_n(t'-t)}{\hbar}\right] \psi_n(\vec{r}) \psi_n^\dagger(\vec{r}') = \sum_n \psi_n(\vec{r}, t) \psi_n^\dagger(\vec{r}', t') \end{aligned} \quad (54)$$

与第一节中哈密顿量不含时定义推导得到的传播子一致。

我们来证明一个单位算符

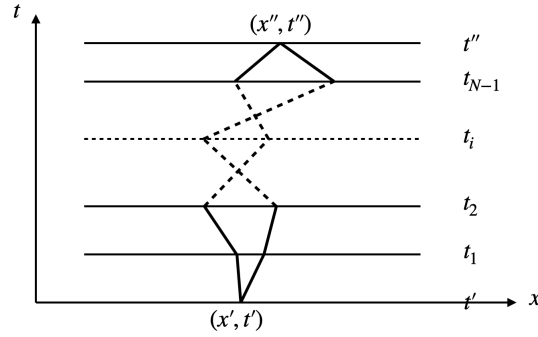
$$\int d\vec{r} |\vec{r}, t\rangle \langle \vec{r}, t| = \int d\vec{r} e^{iHt/\hbar} |\vec{r}\rangle \langle \vec{r}| e^{-iHt/\hbar} = e^{iHt/\hbar} e^{-iHt/\hbar} = 1 \quad (55)$$

$$K(\vec{r}, t; \vec{r}', t') = \langle \vec{r}, t | \vec{r}', t' \rangle = \int d\vec{r}'' \langle \vec{r}, t | \vec{r}'', t'' \rangle \langle \vec{r}'', t'' | \vec{r}', t' \rangle \quad (56)$$

## 4 Feynman's Formulation of Quantum Mechanics

为了书写方便，我们写成一维形式

$$\begin{aligned} & \langle x'', t'' | x', t' \rangle \\ &= \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \langle x'', t'' | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_1, t_1 | x', t' \rangle \end{aligned} \quad (57)$$



粒子从  $(x', t')$  以任意一条路径运动到  $(x'', t'')$

### Dirac's Remark

若  $t_2 \rightarrow t_1$

$$\langle x_2, t_2 | x_1, t_1 \rangle \sim \exp \left[ \frac{i \int_{t_1}^{t_2} L_{\text{classical}}(x, \dot{x}, t) dt}{\hbar} \right] \quad (58)$$

拉格朗日作用量

$$S(n, n-1) = \int_{t_{n-1}}^{t_n} L_{\text{classical}}(x, \dot{x}, t) dt \quad (59)$$

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \sim \exp \left[ \frac{iS(n, n-1)}{\hbar} \right] \quad (60)$$

设  $\Delta t = t_n - t_{n-1} \rightarrow 0$

$$\begin{aligned} S(n, n-1) &= \int_{t_{n-1}}^{t_n} \left[ \frac{m\dot{x}^2}{2} - V(x) \right] dt \\ &= \Delta t \left[ \frac{m}{2} \left( \frac{x_n - x_{n-1}}{\Delta t} \right)^2 - V \left( \frac{x_n + x_{n-1}}{2} \right) \right] \end{aligned} \quad (61)$$

我们可以在  $\langle x'', t'' | x', t' \rangle$  直接放入无穷个积分, 使  $\Delta t$  无穷小

$$\begin{aligned}
& \langle x'', t'' | x', t' \rangle \\
&= \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \langle x'', t'' | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_1, t_1 | x', t' \rangle \\
&\sim \int dx_{N-1} \int dx_{N-2} \cdots \int dx_1 \prod_{n=1}^N \exp \left[ \frac{i}{\hbar} S(n, n-1) \right] \\
&= \int D[x(t)] \exp \left[ \frac{i}{\hbar} \sum_{n=1}^N S(n, n-1) \right] \\
&= \int D[x(t)] \exp \left\{ \frac{i}{\hbar} S_N[x(t)] \right\}
\end{aligned} \tag{62}$$

其中

$$S_N[x(t)] = \sum_{n=1}^N S(n, n-1) = \int_{t'}^{t''} L(x, \dot{x}, t) dt \tag{63}$$

设  $\vec{r}(t_0) = \vec{r}', \vec{r}(t_N) = \vec{r}'', t_0 = t', t_N = t''$ , 且  $t_0, t_1, \dots, t_{N-1}, t_N$  等分

$$\varepsilon = t_j - t_{j-1} \quad j = 1, 2, \dots, N \tag{64}$$

$$S_N[\vec{r}(t)] = \int_{t'}^{t''} L(\vec{r}, \dot{\vec{r}}, t) dt = \varepsilon \sum_{j=1}^N L \left( \frac{\vec{r}_j + \vec{r}_{j-1}}{2}, \frac{\vec{r}_j - \vec{r}_{j-1}}{\varepsilon}, t' + j\varepsilon \right) \tag{65}$$

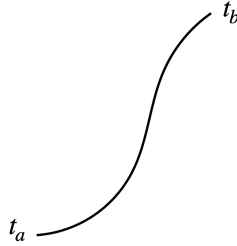
$$K_N(\vec{r}'', t''; \vec{r}', t') = \langle \vec{r}'', t'' | \vec{r}', t' \rangle_N \sim \int D[\vec{r}(t)] \exp \left\{ \frac{i}{\hbar} S_N[\vec{r}(t)] \right\} \tag{66}$$

我们希望

$$K(\vec{r}'', t''; \vec{r}', t') = \lim_{N \rightarrow \infty} K_N(\vec{r}'', t''; \vec{r}', t') \tag{67}$$

## Review: Euler-Lagrange Principle

已知一个粒子  $t_a$  和  $t_b$  时刻的位置, 它的运动轨迹是使作用量  $S[x(t)]$  最小的那一条。



根据最小作用量原理

$$\begin{aligned}
\delta S[x(t)] &= \delta \int_{t_a}^{t_b} L(x, \dot{x}, t) dt \\
&= \int_{t_a}^{t_b} \left( \frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) dt \\
&= \int_{t_a}^{t_b} \left( \frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \frac{d}{dt} \delta x \right) dt \\
&= \int_{t_a}^{t_b} \left[ \frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) \right] \delta x dt + \left[ \frac{\partial L}{\partial \dot{x}} \delta x \right]_{t_a}^{t_b} \\
&= \int_{t_a}^{t_b} \left[ \frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) \right] \delta x dt = 0
\end{aligned} \tag{68}$$

得到 Euler-Lagrange Equation

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = 0 \quad (69)$$

### Example: 1-D Free Particle

$$L = \frac{1}{2} m \dot{x}^2 \quad (70)$$

代入拉格朗日方程

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = 0 \quad (71)$$

得

$$m\dot{x} = \text{constant} \quad (72)$$

$$p = m\dot{x} = m \frac{x'' - x'}{t'' - t'} \quad (73)$$

$$S_N[x(t)] = \int_{t'}^{t''} L(x, \dot{x}, t) dt = \frac{1}{2} \int_{t'}^{t''} m \dot{x}^2 dt = \frac{m}{2} \frac{(x'' - x')^2}{t'' - t'} \quad (74)$$

$$S(x_{j+1}, t_{j+1}; x_j, t_j) = \frac{m}{2} \frac{(x_{j+1} - x_j)^2}{t_{j+1} - t_j} = \frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\varepsilon} \quad (75)$$

由 Dirac's remark 我们知道, 当  $t \rightarrow t'$  时

$$K(x, t; x', t') = C \exp \left[ \frac{iS(x, t; x', t')}{\hbar} \right] = C \exp \left[ \frac{im}{2\hbar} \frac{(x - x')^2}{t - t'} \right] \quad (76)$$

接下来我们用初始条件来定 C。当  $t = t'$  时,

$$K(x, t; x', t') = \delta(x - x') \quad (77)$$

已知积分

$$\lim_{\alpha \rightarrow \infty} e^{-i\alpha x^2} \sqrt{\frac{\alpha}{\pi}} = e^{-\frac{i\pi}{4}} \delta(x) \quad (78)$$

$$\begin{aligned} \lim_{t \rightarrow t'} K(x, t; x', t') &= C \lim_{t \rightarrow t'} \exp \left[ \frac{im}{2\hbar} \frac{(x - x')^2}{t - t'} \right] \\ &= C \lim_{t \rightarrow t'} \exp \left[ \frac{im}{2\hbar} \frac{(x - x')^2}{t - t'} \right] \sqrt{-\frac{m(x - x')^2}{2\pi\hbar(t - t')}} \sqrt{-\frac{2\pi\hbar(t - t')}{m(x - x')^2}} \\ &= C e^{-i\frac{\pi}{4}} \sqrt{-\frac{2\pi\hbar(t - t')}{m(x - x')^2}} \delta(x - x') = \delta(x - x') \end{aligned} \quad (79)$$

$$C = \sqrt{-\frac{m}{2\pi\hbar(t - t')}} e^{i\frac{\pi}{4}} = \sqrt{-\frac{m}{2\pi\hbar(t - t')}} e^{i\frac{\pi}{2}} = \sqrt{\frac{m}{2\pi i\hbar(t - t')}} \quad (80)$$

$$K(x, t; x', t') = C \exp \left[ \frac{im}{2\hbar} \frac{(x - x')^2}{t - t'} \right] = \sqrt{\frac{m}{2\pi i\hbar(t - t')}} \exp \left[ \frac{im}{2\hbar} \frac{(x - x')^2}{t - t'} \right] \quad (81)$$

当  $(t - t')$  为有限大小时, 我们将  $t'$  到  $t$  分成无穷等份

$$\begin{aligned} K(x, t; x', t') &= \int dx_1 \int dx_2 \cdots \int dx_{N-1} \left[ \frac{m}{2\pi i\hbar(t - t')} \right]^{\frac{N}{2}} \exp \left[ \frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2 \right] \\ &= \left[ \frac{m}{2\pi i\hbar(t - t')} \right]^{\frac{N}{2}} \int dx_1 \int dx_2 \cdots \int dx_{N-1} \exp \left[ \frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2 \right] \end{aligned} \quad (82)$$



根据积分

$$\int_{-\infty}^{\infty} dx_2 \exp[\alpha(x_1 - x_2)^2 + \beta(x_3 - x_2)^2] = \exp\left[\frac{\alpha\beta}{\alpha + \beta}(x_1 - x_3)^2\right] \sqrt{-\frac{\pi}{\alpha + \beta}} \quad (83)$$

于是

$$\begin{aligned} & \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left[\frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2\right] \\ &= \left(\frac{2\hbar}{im}\right)^{\frac{N-1}{2}} \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \cdots \int_{-\infty}^{\infty} dy_{N-1} \exp\left[\frac{1}{\varepsilon} \sum_{j=0}^{N-1} (y_{j+1} - y_j)^2\right] \end{aligned} \quad (84)$$

其中  $y = \sqrt{\frac{im}{2\hbar}}x$ 。依次积分，设

$$\alpha_1 = \frac{1}{\varepsilon} \quad \beta = \frac{1}{\varepsilon} \quad \alpha_2 = \frac{\alpha_1\beta}{\alpha_1 + \beta} = \frac{1}{2\varepsilon} \quad \alpha_1 + \beta = \frac{2}{\varepsilon} \quad (85)$$

猜测

$$\alpha_m = \frac{1}{m\varepsilon} \quad (86)$$

则

$$\alpha_{m+1} = \frac{\alpha_m\beta}{\alpha_m + \beta} = \frac{1}{(m+1)\varepsilon} \quad (87)$$

得证。得到普遍表达式

$$\alpha_m + \beta = \frac{1}{m\varepsilon} + \frac{1}{\varepsilon} = \frac{m+1}{m\varepsilon} \quad (88)$$

于是

$$\begin{aligned} & \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left[\frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2\right] \\ &= \left(\frac{2\hbar}{im}\right)^{\frac{N-1}{2}} \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \cdots \int_{-\infty}^{\infty} dy_{N-1} \exp\left[\frac{1}{\varepsilon} \sum_{j=0}^{N-1} (y_{j+1} - y_j)^2\right] \\ &= \left(\frac{2\hbar}{im}\right)^{\frac{N-1}{2}} \exp\left[\frac{1}{N\varepsilon}(y - y')^2\right] \sqrt{-\frac{\pi\varepsilon}{2}} \sqrt{-\frac{\pi 2\varepsilon}{3}} \cdots \sqrt{-\frac{\pi m\varepsilon}{m+1}} \cdots \sqrt{-\frac{\pi(N-1)\varepsilon}{N}} \\ &= \left(\frac{2\hbar}{im}\right)^{\frac{N-1}{2}} \exp\left[\frac{im}{2\hbar} \frac{(x - x')^2}{N\varepsilon}\right] (-\pi\varepsilon)^{\frac{N-1}{2}} \frac{1}{\sqrt{N}} \\ &= \exp\left[\frac{im}{2\hbar} \frac{(x - x')^2}{N\varepsilon}\right] \left(-\frac{2\pi\hbar\varepsilon}{im}\right)^{\frac{N-1}{2}} \frac{1}{\sqrt{N}} \end{aligned} \quad (89)$$

整理成

$$\begin{aligned} K(x, t; x', t') &= \left[\frac{m}{2\pi i\hbar(t-t')}\right]^{\frac{N}{2}} \int dx_1 \int dx_2 \cdots \int dx_{N-1} \exp\left[\frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2\right] \\ &= \left(\frac{m}{2\pi i\hbar N\varepsilon}\right)^{\frac{N}{2}} \exp\left[\frac{im}{2\hbar} \frac{(x - x')^2}{N(t-t')}\right] \left(-\frac{2\pi\hbar\varepsilon}{im}\right)^{\frac{N-1}{2}} \frac{1}{\sqrt{N}} \\ &= \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp\left[\frac{im}{2\hbar} \frac{(x - x')^2}{N(t-t')}\right] \end{aligned} \quad (90)$$

我们发现，用经典理论导出的结果与量子力学的结果完全一致，量子力学是可以从经典理论中导出的。但量子力学和经典力学的过程完全不同，如量子力学中粒子没有固定路线、算符之间的不对易性、海森堡不确定性原理等，都与经典力学完全不一样。过程中发生了什么使得我们通过经典力学的作用量得到量子力学的结果？

回到一维自由粒子情况

$$K(x, t; x', t') = C \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp \left[ \frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2 \right] \quad (91)$$

从中拿出一个积分

$$\begin{aligned} & \int dx_j \exp \left[ \frac{im}{2\hbar\varepsilon} (x_j - x_{j-1})^2 \right] \exp \left[ \frac{im}{2\hbar\varepsilon} (x_{j+1} - x_j)^2 \right] \\ &= \int dx_j \exp \left[ \frac{im}{2\hbar\varepsilon} (x_j^2 - 2x_j x_{j-1} + x_{j-1}^2) \right] \exp \left[ \frac{im}{2\hbar\varepsilon} (x_{j+1}^2 - 2x_{j+1} x_j + x_j^2) \right] \\ &= \exp \left[ \frac{im}{2\hbar\varepsilon} (x_{j-1}^2 + x_{j+1}^2) \right] \exp \left[ -\frac{im}{\hbar\varepsilon} \left( \frac{x_{j-1} - x_{j+1}}{2} \right)^2 \right] \int_{-\infty}^{\infty} dx_j \exp \left[ \frac{im}{\hbar\varepsilon} \left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right)^2 \right] \end{aligned} \quad (92)$$

已知积分

$$\lim_{\alpha \rightarrow \infty} e^{i\alpha x^2} \sqrt{\frac{\alpha}{\pi}} = e^{\frac{i\pi}{4}} \delta(x) \quad (93)$$

当  $\hbar \rightarrow 0$  时, 退化到经典理论, 令  $\alpha = \frac{m}{\hbar\varepsilon} \rightarrow \infty$

$$\begin{aligned} \lim_{\hbar \rightarrow 0} \exp \left[ \frac{im}{\hbar\varepsilon} \left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right)^2 \right] &= \lim_{\alpha \rightarrow \infty} \exp \left[ i\alpha \left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right)^2 \right] \sqrt{\frac{\alpha}{\pi}} \sqrt{\frac{\pi}{\alpha}} \\ &= \sqrt{\frac{\pi\hbar\varepsilon}{m}} e^{\frac{i\pi}{4}} \delta \left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right) \end{aligned} \quad (94)$$

在经典理论中, 积分退化为一点的贡献, 自由粒子的运动路线是一条直线。

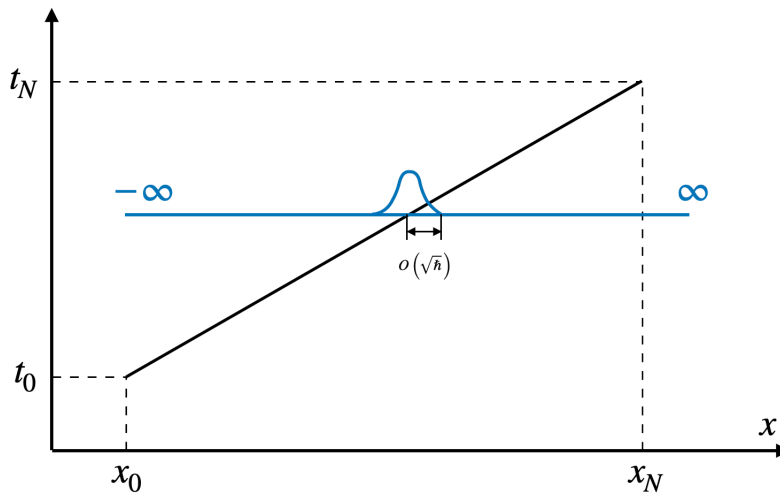
当  $\hbar$  有限时, Gauss 函数有一个很小的贡献

$$\left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right)^2 \frac{m}{\varepsilon \hbar} \sim O(1) \quad (95)$$

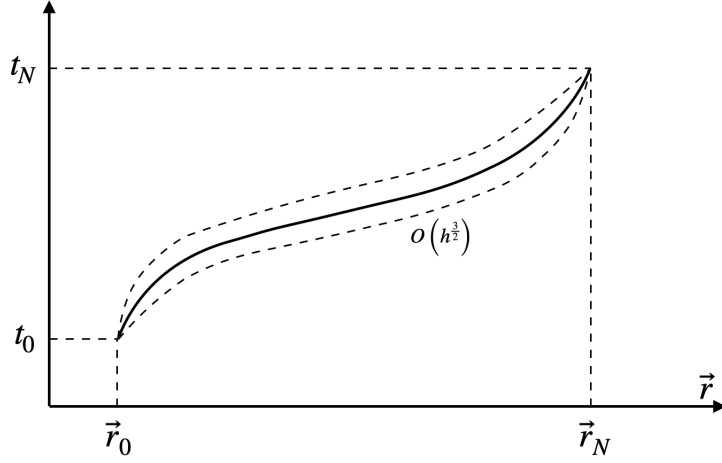
$$\left( x_j - \frac{x_{j-1} + x_{j+1}}{2} \right)^2 \frac{m}{\varepsilon} \sim O(\hbar) \quad (96)$$

$$x_j \sim \frac{x_{j-1} + x_{j+1}}{2} + O(\sqrt{\hbar}) \quad (97)$$

展开宽度的量级是  $\sqrt{\hbar}$ 。



三维情况经典理论下粒子轨迹为一条曲线，而量子力学下有  $\hbar^{\frac{3}{2}}$  的展开宽度。



## 5 从 Feynman 路径积分导出传播子

$$\begin{aligned}
& K(\vec{r}', t'; \vec{r}, t) \\
&= \lim_{N \rightarrow \infty} \int \prod_{j=1}^{N-1} d\vec{r}_j \exp \left\{ \frac{i}{\hbar} S_N[\vec{r}(t)] \right\} \\
&= \lim_{N \rightarrow \infty} \int \prod_{j=1}^{N-1} d\vec{r}_j \exp \left[ \frac{i}{\hbar} \varepsilon \sum_{j=1}^N L \left( \frac{\vec{r}_j + \vec{r}_{j-1}}{2}, \frac{\vec{r}_j - \vec{r}_{j-1}}{\varepsilon}, t + j\varepsilon \right) \right] \\
&= \lim_{M \rightarrow \infty} \lim_{M-N \rightarrow \infty} \int \prod_{j=1}^{M-1} d\vec{r}_j \prod_{i=M+1}^{N-1} d\vec{r}_i d\vec{r}_M \\
&\quad \exp \left\{ \frac{i}{\hbar} \varepsilon \left[ \sum_{j=1}^M L \left( \frac{\vec{r}_j + \vec{r}_{j-1}}{2}, \frac{\vec{r}_j - \vec{r}_{j-1}}{\varepsilon}, t + j\varepsilon \right) + \sum_{i=M+1}^N L \left( \frac{\vec{r}_i + \vec{r}_{i-1}}{2}, \frac{\vec{r}_i - \vec{r}_{i-1}}{\varepsilon}, t + M\varepsilon + i\varepsilon \right) \right] \right\} \quad (98) \\
&= \int d\vec{r}_M \lim_{M \rightarrow \infty} \int \prod_{j=1}^{M-1} d\vec{r}_j \exp \left[ \frac{i}{\hbar} \varepsilon \sum_{j=1}^M L \left( \frac{\vec{r}_j + \vec{r}_{j-1}}{2}, \frac{\vec{r}_j - \vec{r}_{j-1}}{\varepsilon}, t + j\varepsilon \right) \right] \\
&\quad \lim_{N-M \rightarrow \infty} \int \prod_{i=1}^{M-1} d\vec{r}_i \exp \left[ \frac{i}{\hbar} \varepsilon \sum_{i=M}^M L \left( \frac{\vec{r}_i + \vec{r}_{i-1}}{2}, \frac{\vec{r}_i - \vec{r}_{i-1}}{\varepsilon}, t + M\varepsilon + i\varepsilon \right) \right] \\
&= \int d\vec{r}_M K(\vec{r}', t'; \vec{r}_M, t_M) K(\vec{r}_M, t_M; \vec{r}, t)
\end{aligned}$$

$\vec{r}_M$  是赝矢量 (dummy index), 用  $\vec{r}''$  表示  $\vec{r}_M$

$$K(\vec{r}', t'; \vec{r}, t) = \int d\vec{r}'' K(\vec{r}', t'; \vec{r}'', t'') K(\vec{r}'', t''; \vec{r}, t) \quad (99)$$

这个方程我们在薛定谔方程中提到过，现在我们从路径积分中导出同样的结果，验证了这一点。

## 6 Dirac's Remark ( $t_2 \rightarrow t_1$ )

$$\begin{aligned}\langle x_2, t_2 | x_1, t_1 \rangle &\sim \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_2} L(x, \dot{x}, t) dt \right] \\ &= \exp \left\{ \frac{i}{\hbar} \left[ \frac{1}{2} m \frac{(x_2 - x_1)^2}{t_2 - t_1} - (t_2 - t_1) V(x_1) \right] \right\}\end{aligned}\quad (100)$$

在量子力学中我们定义

$$\begin{aligned}\langle x_2, t_2 | x_1, t_1 \rangle &= \langle x_2 | \exp \left[ -\frac{i}{\hbar} H(t_2 - t_1) \right] | x_1 \rangle \\ &= \langle x_2 | \exp \left[ -\frac{i}{\hbar} (H_0 + V)(t_2 - t_1) \right] | x_1 \rangle\end{aligned}\quad (101)$$

$H_0$  和  $V$  在量子力学中具有不对易性, 利用如下关系式

$$\exp[\varepsilon(A + B)] = \exp(\varepsilon A) \exp(\varepsilon B) \left[ \exp\left(-\frac{1}{2}\varepsilon^2[A, B]\right) + O(\varepsilon^3) \right] \quad (102)$$

$$\lim_{\varepsilon \rightarrow 0} \exp[\varepsilon(A + B)] = \exp(\varepsilon A) \exp(\varepsilon B) \quad (103)$$

由于  $(t_2 - t_1) \rightarrow 0$ ,

$$\begin{aligned}\langle x_2, t_2 | x_1, t_1 \rangle &= \langle x_2 | \exp \left[ -\frac{i}{\hbar} H_0(t_2 - t_1) \right] \exp \left[ -\frac{i}{\hbar} V(t_2 - t_1) \right] | x_1 \rangle \\ &= \langle x_2 | \exp \left[ -\frac{i}{\hbar} H_0(t_2 - t_1) \right] | x_1 \rangle \exp \left[ -\frac{i}{\hbar} V(x_1)(t_2 - t_1) \right]\end{aligned}\quad (104)$$

自由粒子的传播子

$$\langle x_2 | \exp \left[ -\frac{i}{\hbar} H_0(t_2 - t_1) \right] | x_1 \rangle = \left[ \frac{m}{2\pi i \hbar (t_2 - t_1)} \right]^{\frac{1}{2}} \exp \left[ \frac{im}{2\hbar} \frac{(x_2 - x_1)^2}{t_2 - t_1} \right] \quad (105)$$

$$\langle x_2, t_2 | x_1, t_1 \rangle = \left[ \frac{m}{2\pi i \hbar (t_2 - t_1)} \right]^{\frac{1}{2}} \exp \left\{ \frac{i}{\hbar} \left[ \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1} - (t_2 - t_1) V(x_1) \right] \right\} \quad (106)$$

当  $t_2 \rightarrow t_1$  时, Feynman 给出的结果和 Schrödinger 给出的结果一致。

## 7 从 Feynman 路径积分导出 $t'' - t' = \text{finite}$ 时的传播子

$$\begin{aligned}\langle x'', t'' | x', t' \rangle &= \langle x'' | \exp \left[ -\frac{i}{\hbar} H(t'' - t') \right] | x' \rangle \\ &= \langle x'' | \exp \left[ -\frac{i}{\hbar} H(t'' - t_{N-1}) \right] \cdots \exp \left[ -\frac{i}{\hbar} H(t_{j+1} - t_j) \right] \cdots \exp \left[ -\frac{i}{\hbar} H(t_1 - t') \right] | x' \rangle \\ &= \int dx_1 \cdots dx_{N-1} \langle x'' | \exp \left[ -\frac{i}{\hbar} H(t'' - t_{N-1}) \right] | x_{N-1} \rangle \cdots \\ &\quad \langle x_{j+1} | \exp \left[ -\frac{i}{\hbar} H(t_{j+1} - t_j) \right] | x_j \rangle \cdots \langle x_1 | \exp \left[ -\frac{i}{\hbar} H(t_1 - t') \right] | x' \rangle \\ &= \left( \frac{m}{2\pi i \hbar \varepsilon} \right)^{\frac{N}{2}} \int dx_1 \cdots dx_{N-1} \exp \left\{ \sum_{j=1}^{N-1} \left[ \frac{im(x_{j+1} - x_j)^2}{2\hbar \varepsilon} - \frac{i}{\hbar} \varepsilon V(x_j) \right] \right\} \\ &= \int D[x(t)] \exp \left\{ \frac{i}{\hbar} \int_{t'}^{t''} \left[ \frac{m}{2} \dot{x}^2 - V(x) \right] dt \right\}\end{aligned}\quad (107)$$

根据 Lie-Trotter Formula

$$\exp[it(A+B)] = \lim_{N \rightarrow \infty} \left[ \exp\left(\frac{itA}{N}\right) \exp\left(\frac{itB}{N}\right) \right]^N \quad (108)$$

$$\begin{aligned} & \langle x | \exp\left[-\frac{i}{\hbar} H(t-t')\right] | x' \rangle \\ &= \langle x | \exp\left[-\frac{i}{\hbar} (H_0 + V)(t-t')\right] | x' \rangle \\ &= \langle x | \left[ \exp\left(-\frac{iH_0\varepsilon}{\hbar}\right) \exp\left(-\frac{iV\varepsilon}{\hbar}\right) \right]^N | x' \rangle \\ &= \int dx_1 \cdots dx_{N-1} \langle x'' | \exp\left(-\frac{iH_0\varepsilon}{\hbar}\right) \exp\left(-\frac{iV\varepsilon}{\hbar}\right) | x_{N-1} \rangle \cdots \langle x_1 | \exp\left(-\frac{iH_0\varepsilon}{\hbar}\right) \exp\left(-\frac{iV\varepsilon}{\hbar}\right) | x' \rangle \end{aligned} \quad (109)$$

$$\begin{aligned} &= \langle x_N = x | \prod_{j=1}^{N-1} \int_{-\infty}^{\infty} dx_j \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] | x_{N-1} \rangle \langle x_{N-1} | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \\ & \quad \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] | x_{N-2} \rangle \cdots | x_1 \rangle \langle x_1 | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] | x_1 = x' \rangle \\ &= \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N}{2}} \prod_{j=1}^{N-1} \int_{-\infty}^{\infty} dx_j \exp\left[\frac{i}{\hbar} \int_{t'}^t L dt''\right] \\ & \quad K(x, t, x', t') = \int D[x(t)] \exp\left[\frac{i}{\hbar} S(t, t')\right] \end{aligned} \quad (110)$$

我们可以从 Feynman 路径积分给出量子力学的结果。

## 8 从 Feynman 路径积分导出传播子的运动方程

已知运动方程

$$i\hbar \frac{\partial}{\partial t} \langle x, t | x', t' \rangle = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \langle x, t | x', t' \rangle \quad (111)$$

$$\begin{aligned} \langle x, t | x', t' \rangle &\sim \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N}{2}} \prod_{j=1}^{N-1} \int dx_j \exp\left[\frac{i}{\hbar} S(t, t')\right] \\ &= \left[\frac{m}{2\pi i\hbar(t-t_{N-1})}\right]^{\frac{1}{2}} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{N-1}{2}} \prod_{j=1}^{N-1} \int dx_j \exp\left[\frac{i}{\hbar} S(t, t_{N-1})\right] \prod_{n=1}^{N-1} \exp\left[\frac{i}{\hbar} S(n, n-1)\right] \end{aligned} \quad (112)$$

方程左边

$$i\hbar \frac{\partial}{\partial t} \langle x, t | x', t' \rangle = i\hbar \left(-\frac{1}{2}\right) \frac{1}{t-t_{N-1}} \langle x, t | x', t' \rangle - \left[\frac{\partial}{\partial t} S(t, t_{N-1})\right] \langle x, t | x', t' \rangle \quad (113)$$

其中

$$\begin{aligned} \frac{\partial}{\partial t} S(t, t_{N-1}) &= \frac{\partial}{\partial t} \left[ (t-t_{N-1}) L\left(\frac{x+x_{N-1}}{2}, \frac{x-x_{N-1}}{t-t_{N-1}}, \frac{t+t_{N-1}}{2}\right) \right] \\ &= \frac{\partial}{\partial t} \left\{ (t-t_{N-1}) \left[ \frac{1}{2} m \left(\frac{x-x_{N-1}}{t-t_{N-1}}\right)^2 - V\left(\frac{x+x_{N-1}}{2}\right) \right] \right\} \\ &= -\frac{1}{2} m \left(\frac{x-x_{N-1}}{t-t_{N-1}}\right)^2 - V\left(\frac{x+x_{N-1}}{2}\right) \\ &= -T - V \end{aligned} \quad (114)$$

代回 Eq.(113)

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle x, t|x', t' \rangle &= i\hbar \left( -\frac{1}{2} \right) \frac{1}{t - t_{N-1}} \langle x, t|x', t' \rangle - \left[ \frac{\partial}{\partial t} S(t, t_{N-1}) \right] \langle x, t|x', t' \rangle \\ &= \left[ i\hbar \left( -\frac{1}{2} \right) \frac{1}{t - t_{N-1}} + \frac{1}{2} m \left( \frac{x - x_{N-1}}{t - t_{N-1}} \right)^2 + V(x) \right] \langle x, t|x', t' \rangle \end{aligned} \quad (115)$$

方程右边

$$\text{RHS} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \langle x, t|x', t' \rangle \quad (116)$$

其中

$$\begin{aligned} \frac{\partial}{\partial x} \langle x, t|x', t' \rangle &= \frac{i}{\hbar} \langle x, t|x', t' \rangle \frac{\partial}{\partial x} S(t, t_{N-1}) \\ &= \frac{i}{\hbar} \langle x, t|x', t' \rangle \frac{\partial}{\partial x} \left\{ (t - t_{N-1}) \left[ \frac{1}{2} m \left( \frac{x - x_{N-1}}{t - t_{N-1}} \right)^2 - V \left( \frac{x + x_{N-1}}{2} \right) \right] \right\} \\ &= \frac{im}{\hbar} \frac{x - x_{N-1}}{t - t_{N-1}} \langle x, t|x', t' \rangle \end{aligned} \quad (117)$$

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \langle x, t|x', t' \rangle &= \frac{\partial}{\partial x} \left( \frac{im}{\hbar} \frac{x - x_{N-1}}{t - t_{N-1}} \langle x, t|x', t' \rangle \right) \\ &= \left[ \frac{im}{\hbar} \frac{1}{t - t_{N-1}} - \frac{m^2}{\hbar^2} \left( \frac{x - x_{N-1}}{t - t_{N-1}} \right)^2 \right] \langle x, t|x', t' \rangle \end{aligned} \quad (118)$$

$$\begin{aligned} \text{RHS} &= \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \langle x, t|x', t' \rangle \\ &= \left[ -\frac{i\hbar}{2} \frac{1}{t - t_{N-1}} + \frac{m}{2} \left( \frac{x - x_{N-1}}{t - t_{N-1}} \right)^2 + V(x) \right] \langle x, t|x', t' \rangle \end{aligned} \quad (119)$$

LHS=RHS, 故运动方程得证。即可以通过 Feynman 路径积分导出运动方程。

## 9 Equivalence of Feynman's Formulation and Schrödinger Function

$$\psi(x, t + \varepsilon) = \int_{-\infty}^{\infty} K(x, t + \varepsilon, y, t) \psi(y, t) dy \quad (120)$$

Dirac's remark 给出, 当  $\varepsilon \rightarrow 0^+$  时

$$K(x, t + \varepsilon, y, t) = C \exp \left[ \frac{i\varepsilon}{\hbar} L \left( \frac{x + y}{2}, \frac{x - y}{\varepsilon}, t \right) \right] = C \exp \left\{ \frac{i\varepsilon}{\hbar} \left[ \frac{m}{2} \left( \frac{x - y}{\varepsilon} \right)^2 - V \left( \frac{x + y}{2}, t \right) \right] \right\} \quad (121)$$

代回 Eq.(120)

$$\psi(x, t + \varepsilon) = C \int_{-\infty}^{\infty} \exp \left\{ \frac{i\varepsilon}{\hbar} \left[ \frac{m}{2} \left( \frac{x - y}{\varepsilon} \right)^2 - V \left( \frac{x + y}{2}, t \right) \right] \right\} \psi(y, t) dy \quad (122)$$

令  $x = y - \eta$

$$\psi(x, t + \varepsilon) = C \int_{-\infty}^{\infty} d\eta \exp \left\{ \frac{i\varepsilon}{\hbar} \left[ \frac{m\eta^2}{2\varepsilon^2} - V \left( x + \frac{\eta}{2}, t \right) \right] \right\} \psi(x + \eta, t) \quad (123)$$

展开

$$\psi(x, t) + \varepsilon \frac{\partial}{\partial t} \psi = C \int_{-\infty}^{\infty} d\eta \exp \left( \frac{im\eta^2}{2\hbar\varepsilon} \right) \exp \left[ -\frac{i\varepsilon}{\hbar} V \left( x + \frac{\eta}{2}, t \right) \right] \left[ \psi(x, t) + \eta \frac{\partial}{\partial x} \psi + \frac{1}{2} \eta^2 \frac{\partial^2}{\partial x^2} \psi + \cdots \right] \quad (124)$$

由于

$$\frac{m\eta^2}{2\hbar\varepsilon} \sim O(1) \quad \eta \sim O(\sqrt{\varepsilon}) \quad (125)$$

$\varepsilon$  和  $\eta$  是小量

$$\psi(x, t) + \varepsilon \frac{\partial}{\partial t} \psi = C \int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \left[1 - \frac{i\varepsilon}{\hbar} V(x, t)\right] \left[\psi(x, t) + \eta \frac{\partial}{\partial x} \psi + \frac{1}{2} \eta^2 \frac{\partial^2}{\partial x^2} \psi + \cdots\right] \quad (126)$$

已知积分

$$\int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) = \sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \quad (127)$$

$$\int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \eta = 0 \quad (128)$$

$$\int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \eta^2 = \frac{\sqrt{\pi}}{2} \left(\frac{2\hbar\varepsilon i}{m}\right)^{\frac{3}{2}} \quad (129)$$

则

$$C \sqrt{\frac{2\pi\hbar\varepsilon i}{m}} = 1 \quad \Rightarrow \quad C = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \quad (130)$$

$$C \int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \eta^2 = \frac{\sqrt{\pi}}{2} \left(\frac{2\hbar\varepsilon i}{m}\right)^{\frac{3}{2}} \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} = \frac{i\hbar\varepsilon}{m} \quad (131)$$

$$\begin{aligned} \psi(x, t) + \varepsilon \frac{\partial}{\partial t} \psi &= C \int_{-\infty}^{\infty} d\eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \left[1 - \frac{i\varepsilon}{\hbar} V(x, t)\right] \left[\psi(x, t) + \eta \frac{\partial}{\partial x} \psi + \frac{1}{2} \eta^2 \frac{\partial^2}{\partial x^2} \psi + \cdots\right] \\ &= \left[1 - \frac{i\varepsilon}{\hbar} V(x, t)\right] \left[\psi(x, t) + \frac{1}{2} \frac{\partial^2}{\partial x^2} \psi(x, t) \frac{i\hbar\varepsilon}{m}\right] \end{aligned} \quad (132)$$

整理得

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t)\right] \psi(x, t) \quad (133)$$

## 10 Formulation in the Phase Space

$$\begin{aligned}
& K(x, t; x', t') \\
&= \int \prod_{j=1}^{N-1} dx_j \langle x | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x_{N-1}\rangle \langle x_{N-1}| \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x_{N-2}\rangle \cdots \\
&\quad \langle x_1 | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x'\rangle \\
&= \int \prod_{j=1}^{N-1} dx_j \prod_{i=1}^N dp_i \langle x | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) |p_N\rangle \langle p_N| \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x_{N-1}\rangle \langle x_{N-1}| \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) |p_{N-1}\rangle \\
&\quad \langle p_{N-1}| \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x_{N-2}\rangle \cdots \langle x_1 | \exp\left(-\frac{i\varepsilon}{2m\hbar} p^2\right) |p_1\rangle \langle p_1| \exp\left[-\frac{i\varepsilon}{\hbar} V(x)\right] |x'\rangle \\
&= \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^{2N} \int \prod_{j=1}^{N-1} dx_j \prod_{i=1}^N dp_i \exp\left(-\frac{i\varepsilon}{2m\hbar} p_N^2\right) \exp\left(\frac{ip_N x_N}{\hbar}\right) \exp\left(-\frac{ip_N x_{N-1}}{\hbar}\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x_{N-1})\right] \\
&\quad \exp\left(-\frac{i\varepsilon}{2m\hbar} p_{N-1}^2\right) \exp\left(\frac{ip_{N-1} x_{N-1}}{\hbar}\right) \exp\left(-\frac{ip_{N-1} x_{N-2}}{\hbar}\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x_{N-2})\right] \cdots \\
&\quad \exp\left(-\frac{i\varepsilon}{2m\hbar} p_1^2\right) \exp\left(\frac{ip_1 x_1}{\hbar}\right) \exp\left(-\frac{ip_1 x'}{\hbar}\right) \exp\left[-\frac{i\varepsilon}{\hbar} V(x')\right] \\
&= \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^{2N} \int \prod_{j=1}^{N-1} dx_j \prod_{i=1}^N dp_i \exp\left\{\frac{i\varepsilon}{\hbar} \left[p_i \frac{x_i - x_{i-1}}{\varepsilon} - \frac{p_i^2}{2m} - V(x_{i-1})\right]\right\} \\
&= \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^{2N} \int \prod_{j=1}^{N-1} dx_j \prod_{i=1}^N dp_i \exp\left[\frac{i\varepsilon}{\hbar} (p_i \dot{x} - H)\right] \\
&= \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^{2N} \int \prod_{j=1}^{N-1} dx_j \prod_{i=1}^N dp_i \exp\left(\frac{iS}{\hbar}\right)
\end{aligned} \tag{134}$$

$$K(x, t; x', t') = \int D[x] D[p] \exp\left(\frac{iS}{\hbar}\right) \tag{135}$$

## 11 从 Feynman 路径积分导出 $K(x, t; x', t') = \delta(x - x')$ ( $t \rightarrow t'$ )

$$K(x, t; x', t') = \int dx_1 \int dx \cdots \int dx_{N-1} \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{\frac{N}{2}} \exp\left[\frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2\right] \tag{136}$$

$$\lim_{\varepsilon \rightarrow 0} \exp\left[\frac{im}{2\hbar\varepsilon} (x_{j+1} - x_j)^2\right] = \sqrt{-\frac{2\pi\hbar\varepsilon}{m}} e^{-\frac{i\pi}{4}} \delta(x_{j+1} - x_j) \tag{137}$$

$$\begin{aligned}
K(x, t; x', t') &= \int dx_1 \int dx \cdots \int dx_{N-1} \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{\frac{N}{2}} \exp\left[\frac{im}{2\hbar\varepsilon} \sum_{j=0}^{N-1} (x_{j+1} - x_j)^2\right] \\
&= \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{\frac{N}{2}} \left(-\frac{2\pi\hbar\varepsilon}{m}\right)^{\frac{N}{2}} \left(e^{-\frac{i\pi}{4}}\right)^N \int dx_1 \int dx \cdots \int dx_{N-1} \prod_{j=0}^{N-1} \delta(x_{j+1} - x_j) \\
&= (i)^{\frac{N}{2}} \left(e^{-\frac{i\pi}{2}}\right)^{\frac{N}{2}} \delta(x - x') = \delta(x - x')
\end{aligned} \tag{138}$$



## 12 从 Feynman 路径积分导出 Time-dependent Case 的结论

$$|\psi(t)\rangle = U(t, t') |\psi(t')\rangle \quad (139)$$

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H(t)U(t, t') \quad (140)$$

设  $H(t) = H$  时的解是

$$U(t, t') = \exp\left[-\frac{iH(t-t')}{\hbar}\right] \quad (141)$$

接下来求  $U(t, t')$  的形式解

$$dU(t, t') = \frac{1}{i\hbar} H(t)U(t, t')dt \quad (142)$$

$$\int_{t'}^{t''} dU(t, t') = \frac{1}{i\hbar} \int_{t'}^{t''} H(t)U(t, t')dt \quad (143)$$

由于  $U(t', t') = 1$ , 得到

$$U(t'', t') - 1 = \frac{1}{i\hbar} \int_{t'}^{t''} H(t)U(t, t')dt \quad (144)$$

$$\begin{aligned} U(t'', t') &= 1 + \frac{1}{i\hbar} \int_{t'}^{t''} H(t_1)U(t_1, t')dt_1 \\ &= 1 + \frac{1}{i\hbar} \int_{t'}^{t''} H(t_1) \left[ 1 + \frac{1}{i\hbar} \int_{t'}^{t_1} H(t_2)U(t_2, t')dt_2 \right] dt_1 \\ &= 1 + \frac{1}{i\hbar} \int_{t'}^{t''} H(t_1)dt_1 + \left( \frac{1}{i\hbar} \right)^2 \int_{t'}^{t''} dt_1 \int_{t'}^{t_1} dt_2 H(t_1)H(t_2)U(t_2, t') \\ &= \dots \\ &= 1 + \sum_{n=1}^{\infty} \left( \frac{1}{i\hbar} \right)^n \int_{t'}^{t''} dt_1 \int_{t'}^{t_1} dt_2 \dots \int_{t'}^{t_{n-1}} dt_n H(t_1)H(t_2) \dots H(t_n) \\ &= (t'' - t') \exp \left[ -\frac{i}{\hbar} \int_{t'}^{t''} dt H(t) \right] \end{aligned} \quad (145)$$

故

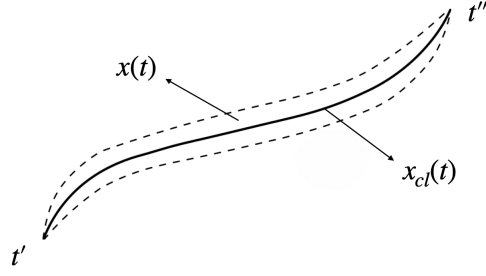
$$U(t, t') = T \exp \left[ -\frac{i}{\hbar} \int_{t'}^t dt'' H(t'') \right] \quad (146)$$

## 13 General Method for Calculating the Propagator (Semiclassical Method)

$$K(x'', t''; x', t') = \int D[x(t)] e^{\frac{i}{\hbar} S} \quad (147)$$

其中

$$S = \int_{t'}^{t''} dt L(x, \dot{x}, t) = \int_{t'}^{t''} dt \left[ \frac{1}{2} m \dot{x}^2 - V(x, t) \right] \quad (148)$$



$$x(t) = x_{\text{cl}}(t) + q(t) \quad (149)$$

其中  $q(t)$  来源于量子涨落 (QM-Fluctuation), 是小量,  $x_{\text{cl}}(t)$  满足

$$\frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{x}_{\text{cl}}} \right) - \frac{\partial L}{\partial x_{\text{cl}}} = 0 \quad (150)$$

$$\dot{x}(t) = \dot{x}_{\text{cl}}(t) + \dot{q}(t) \quad \dot{q}(t') = \dot{q}(t'') \quad (151)$$

$$\begin{aligned} S &= \int_{t'}^{t''} dt \left[ \frac{1}{2} m (\dot{x}_{\text{cl}} + \dot{q})^2 - V(x_{\text{cl}} + q, t) \right] \\ &= \int_{t'}^{t''} dt \left[ \frac{1}{2} m (\dot{x}_{\text{cl}}^2 + 2\dot{x}_{\text{cl}}\dot{q} + \dot{q}^2) - V(x_{\text{cl}}, t) - \frac{\partial V}{\partial x_{\text{cl}}} q \right] \\ &= S_{\text{cl}} + \int_{t'}^{t''} dt \left[ \frac{1}{2} m (2\dot{x}_{\text{cl}}\dot{q} + \dot{q}^2) - \frac{\partial V}{\partial x_{\text{cl}}} q \right] \end{aligned} \quad (152)$$

由于

$$\int_{t'}^{t''} dt \frac{d}{dt} (\dot{x}q) = \int_{t'}^{t''} dt (\ddot{x}q + \dot{x}\dot{q}) = 0 \quad (153)$$

则

$$\dot{x}\dot{q} = -\ddot{x}q \quad (154)$$

$$S = S_{\text{cl}} + \int_{t'}^{t''} dt \left[ \frac{1}{2} m (-2\ddot{x}q + \dot{q}^2) - \frac{\partial V}{\partial x_{\text{cl}}} q \right] \quad (155)$$

又

$$m\ddot{x}_{\text{cl}} = -\frac{\partial V}{\partial x_{\text{cl}}} \quad (156)$$

$$S = S_{\text{cl}} + \int_{t'}^{t''} dt \left( \frac{1}{2} m \dot{q}^2 - \frac{1}{2} \frac{\partial^2 V}{\partial x_{\text{cl}}^2} q^2 \right) = S_{\text{cl}} + S_{\text{QM-F}} \quad (157)$$

量子涨落

$$\begin{aligned} S_{\text{QM-F}} &= \int_{t'}^{t''} dt \left( \frac{1}{2} m \dot{q}^2 - \frac{1}{2} \frac{\partial^2 V}{\partial x_{\text{cl}}^2} q^2 \right) \\ &= \frac{m}{2} \int_{t'}^{t''} dt q \left( -\frac{d^2}{dt^2} - \frac{1}{m} \frac{\partial^2 V}{\partial x_{\text{cl}}^2} \right) q \\ &= \frac{m}{2} \int_{t'}^{t''} dt q(t) A(t) q(t) \end{aligned} \quad (158)$$

其中

$$A(t) = -\frac{d^2}{dt^2} - \frac{1}{m} \frac{\partial^2 V}{\partial x_{\text{cl}}^2} = -\frac{d^2}{dt^2} - \omega(t) \quad (159)$$

$$\omega(t) = \frac{1}{m} \frac{\partial^2 V}{\partial x_{\text{cl}}^2} \quad (160)$$

$A(t)$  是厄米算符

$$A(t)\varphi_n(t) = \lambda_n\varphi_n(t) \quad (161)$$

$\varphi_n(t)$  构成完备基, 用  $\varphi_n(t)$  展开  $q(t)$

$$q(t) = \sum_{n=1}^{\infty} a_n \varphi_n(t) = \lim_{N \rightarrow \infty} \sum_{n=1}^N a_n \varphi_n(t) \quad (162)$$

$$\begin{aligned} S_{\text{QM-F}} &= \frac{m}{2} \sum_{n,m} \int_{t'}^{t''} dt a_n a_m \varphi_n(t) A(t) \varphi_m(t) \\ &= \frac{m}{2} \sum_{n,m} a_n a_m \int_{t'}^{t''} dt \varphi_n(t) A(t) \varphi_m(t) \\ &= \frac{m}{2} \sum_{n,m} a_n a_m \lambda_m \int_{t'}^{t''} dt \varphi_n(t) \varphi_m(t) \\ &= \frac{m}{2} \sum_{n,m} a_n a_m \lambda_m \delta_{m,n} T \\ &= \frac{m}{2} \sum_n a_n^2 \lambda_n T \end{aligned} \quad (163)$$

$$\begin{aligned} K(x'', t''; x', t') &= \int D[x(t)] e^{\frac{i}{\hbar} S} \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \int D[q(t)] e^{\frac{i}{\hbar} S_{\text{QM-F}}} \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \int D[q(t)] \exp\left(\frac{im}{2\hbar} \sum_n a_n^2 \lambda_n T\right) \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \pi^N N! \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{N+1}{2}} \int \prod_{n=1}^N da_n \exp\left(\frac{im}{2\hbar} \sum_n a_n^2 \lambda_n T\right) \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \pi^N N! \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{N+1}{2}} \left(\frac{2\pi \hbar i}{mT}\right)^{\frac{N}{2}} \frac{1}{\sqrt{\prod_{n=1}^N \lambda_n}} \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \pi^N N! \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{1}{2}} T^{-N} \frac{1}{\sqrt{\prod_{n=1}^N \lambda_n}} \end{aligned} \quad (164)$$

**Example: 1-D Free Particle**

$$\lambda_n = \left(\frac{n\pi}{T}\right)^2 \quad (165)$$

$$\prod_{n=1}^N \lambda_n = \prod_{n=1}^N \left(\frac{n\pi}{T}\right)^2 = (N!)^2 \frac{\pi^{2N}}{T^{2N}} \quad (166)$$

$$\begin{aligned} K(x'', t''; x', t') &= e^{\frac{i}{\hbar} S_{\text{cl}}} \pi^N N! \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{1}{2}} T^{-N} \frac{1}{\sqrt{\prod_{n=1}^N \lambda_n}} \\ &= e^{\frac{i}{\hbar} S_{\text{cl}}} \pi^N N! \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{1}{2}} T^{-N} \frac{T^N}{N! \pi^N} \\ &= \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} S_{\text{cl}}} \end{aligned} \quad (167)$$