Numerical Path Integral

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June 2, 2025

Contents

1 path integral in quantum mechanics

- 考虑系统的 Hamiltonian 为

$$H = \frac{p^2}{2m} + V(x), \tag{1.1}$$

那么其 Lagrangian 为

$$L = \frac{m}{2}\dot{x}^2 - V(x), \tag{1.2}$$

系统初态为 $|\psi_0\rangle$.

- 用 path integral 计算 $\psi(T,x) = \langle x|e^{-iHT}|\psi_0\rangle$, 有

$$\begin{aligned}\langle x|e^{-iHT}|\psi_0\rangle &= \int Dx\, e^{i\int_0^T dt\, L} \\ &= \lim_{N\to\infty} \int dx_0\, \psi_0(x_0) \int dx_{N+1}\, \delta(x_{N+1} - x) \\ &\quad \int dx_1 \cdots dx_N\, \exp\Big(i\sum_{i=0}^{N} \Delta t\Big(\frac{m}{2}\Big(\frac{x_{i+1}-x_i}{\Delta t}\Big)^2 - V(x_i)\Big)\Big),\end{aligned} \tag{1.3}$$

其中 $\Delta t = \frac{T}{N+1}$.

- 数値计算中, 令

$$\begin{cases} x_i = \Big(\dfrac{2i}{M} - 1\Big)L, \Delta x = \dfrac{2L}{M}, i = 0, \cdots, M \\ K_{ij} = \langle x_i|e^{-iH\Delta t}|x_j\rangle = \sqrt{\dfrac{m}{2\pi i \Delta t}} \exp\Big(i\Big(\dfrac{m}{2}\dfrac{(x_i-x_j)^2}{\Delta t} - \Delta t V(x_i)\Big)\Big) \end{cases}, \tag{1.4}$$

那么

$$\langle x|e^{-iHT}|\psi_0\rangle = \lim_{L,M,N\to\infty} (\Delta x)^{N+1} \sum_{j=0}^{M} (K^{N+1})_{ij}\psi_0(x_j), \quad \text{with} \quad x_i = x \ll L. \tag{1.5}$$

1.1 Gaussian wave packet

- 考虑一个自由粒子, 初态为

$$\psi_0(x) = \Big(\frac{2}{\pi}\Big)^{\frac{1}{4}} e^{-x^2 + ik_0 x}, \quad \langle k|\psi_0\rangle = \frac{1}{(2\pi)^{1/4}} e^{-\frac{1}{4}(k-k_0)^2}, \tag{1.6}$$

那么, 预期结果为

$$\psi(t,x)=\left(\frac{2}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{m}{m+2it}}\exp\left(\frac{m}{m+2it}(-x^2+ik_0x)-i\frac{k_0^2}{2(m+2it)}t\right). \tag{1.7}$$

- 计算 (1.5) 最快 (且节省内存) 的方法是 (每一步计算都得到向量, 而不是矩阵):

```
psi_final = psi_0
for i in range(N+1):
        psi_final = dx * K @ psi_final
```

不推荐以下两种方法 (在 $T=0.1, L=300, M=9000, N=1$ 时可以得到较准确的波形):

```
K_power = K
for i in range(N):
        K_power = K @ K_power
psi_final = dx**(N + 1) * K_power @ psi_0
```

或

```
K_power = np.linalg.matrix_power(K, N + 1)
psi_final = dx**(N + 1) * K_power @ psi_0
```

- 另外, 根据经验, 需要有 $\left|\Delta x\sqrt{\frac{m}{2\pi i\Delta t}}\right|^2 \ll 1$, 可以选取 $\sim 10^{-2}$.
- 令 $m=k_0=1$, 数值计算得到的结果如下图所示 (其中 $A=\int dx\,\rho$ 是数值计算得到的 normalization constant):

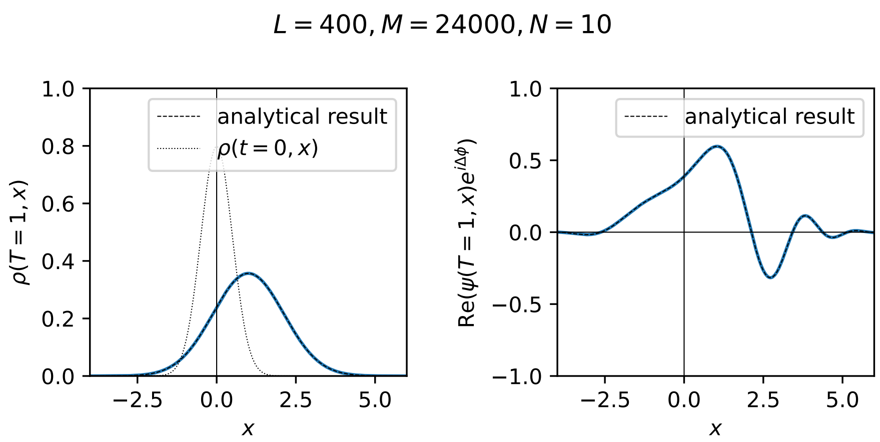

Figure 1: numerical path integral (normalized) at $T=1$ with $A\sim 10^{18}, \Delta\phi\approx\pi+0.7$.

1.2 harmonic oscillator and coherent states

- 考虑谐振子的 coherent states,

$$\begin{cases}\psi^{(\alpha)}(t,x)=\left(\frac{m\omega}{\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega}{2}(x-\langle x\rangle)^2+i\langle p\rangle x+i\theta(t)\right)\\ \langle x\rangle=\sqrt{\frac{2}{m\omega}}\mathrm{Re}(\alpha e^{-i\omega t}), \langle p\rangle=\sqrt{2m\omega}\mathrm{Im}(\alpha e^{-i\omega t})\\ \theta(t)=-\frac{\omega t}{2}-\mathrm{Re}(\alpha e^{-i\omega t})\mathrm{Im}(\alpha e^{-i\omega t})\end{cases}, \tag{1.8}$$

其中 $\alpha\in\mathbb{C}$.

- 令 $m=\omega=1$, 考虑初始条件为 $\alpha=|\alpha|=1$ 的情况. 计算中可以让

$$K_{ij}=\sqrt{\frac{m}{2\pi i\Delta t}}\exp\left(i\frac{m}{2}\frac{(x_i-x_j)^2}{\Delta t}\right)\frac{e^{-i\Delta tV(x_i)}+e^{-i\Delta tV(x_j)}}{2}, \tag{1.9}$$

这对数值结果有微小的改进.

- 数值计算结果如下:

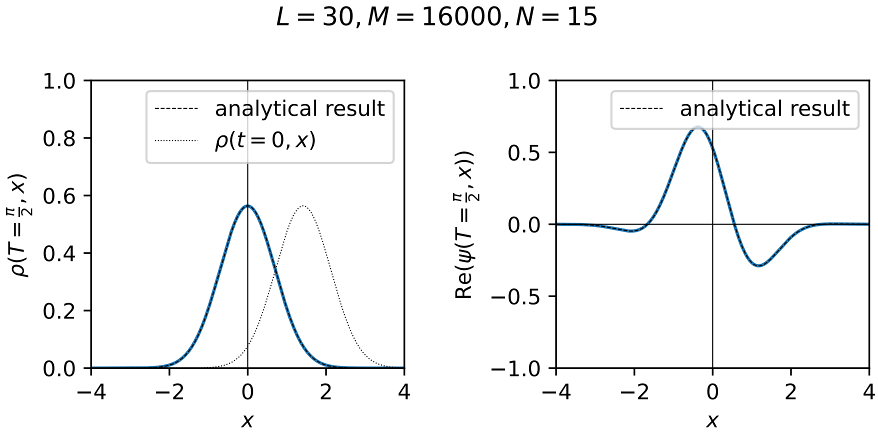

Figure 2: numerical path integral at $T = \frac{\pi}{2}$.

注意到, coherent state 用路径积分数值计算得到的结果具有正确的归一化系数 $A = 1$ 和相位.

A coherent states

- 参考: Wikipedia: Coherent state, Wikipedia: Displacement operator.
- coherent states, $|\alpha\rangle$, 是 annihilation operator 的本征态

$$\begin{cases} a\,|\alpha\rangle = \alpha\,|\alpha\rangle\,, \alpha \in \mathbb{C} \\ |\alpha\rangle = D(\alpha)\,|0\rangle \end{cases}, \tag{A.1}$$

其中 $D(\alpha)$ 是 displacement operator,

$$D(\alpha) := e^{\alpha a^\dagger - \alpha^* a}. \tag{A.2}$$

calculation:

$$\begin{cases} [a, (\alpha a^\dagger - \alpha^* a)^n] = n\alpha(\alpha a^\dagger - \alpha^* a)^{n-1} \\ [a^\dagger, (\alpha a^\dagger - \alpha^* a)^n] = n\alpha^*(\alpha a^\dagger - \alpha^* a)^{n-1} \\ [a^\dagger a, (\alpha a^\dagger - \alpha^* a)^n] = n(\alpha a^\dagger + \alpha^* a)(\alpha a^\dagger - \alpha^* a)^{n-1} - n(n-1)|\alpha|^2(\alpha a^\dagger - \alpha^* a)^{n-2} \end{cases}$$
$$\Longrightarrow \begin{cases} [a, e^{\alpha a^\dagger - \alpha^* a}] = \alpha e^{\alpha a^\dagger - \alpha^* a} \\ [a^\dagger, e^{\alpha a^\dagger - \alpha^* a}] = \alpha^* e^{\alpha a^\dagger - \alpha^* a} \\ [a^\dagger a, e^{\alpha a^\dagger - \alpha^* a}] = (\alpha a^\dagger + \alpha^* a - |\alpha|^2) e^{\alpha a^\dagger - \alpha^* a} \end{cases}, \tag{A.3}$$

因此

$$\begin{cases} a\,|\alpha\rangle = \cdots \\ a^\dagger\,|\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a}\,|1\rangle + \alpha^*\,|\alpha\rangle \\ a^\dagger a\,|\alpha\rangle = \alpha a^\dagger\,|\alpha\rangle \Longrightarrow \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2\,\langle\alpha|\alpha\rangle \end{cases}. \tag{A.4}$$

- displacement operator 是 unitary operator, 且满足

$$\begin{cases} D(\alpha) := e^{\alpha a^\dagger - \alpha^* a} = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\frac{1}{2}|\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger} \\ D(\alpha)D(\beta) = e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} D(\alpha + \beta) \\ D^\dagger(\alpha) = D(-\alpha) \\ D^\dagger(\alpha) a D(\alpha) = a + \alpha \\ D^\dagger(\alpha) a^\dagger D(\alpha) = a^\dagger + \alpha^* \end{cases}. \tag{A.5}$$

calculation:

首先

$$D^\dagger(\alpha) = \sum_{n=0}^{\infty} \frac{1}{n!}((\alpha a^\dagger - \alpha^* a)^\dagger)^n = \sum_{n=0}^{\infty} \frac{1}{n!}(\alpha^* a - \alpha a^\dagger)^n = D(-\alpha), \tag{A.6}$$

使用 BCH formula,

$$\begin{cases} e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] - \frac{1}{12}[B,[A,B]] + \cdots\right) \\ e^A B e^{-A} = e^{\mathrm{ad}_A} B \end{cases}$$

$$\Longrightarrow \begin{cases} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\alpha a^\dagger - \alpha^* a + \frac{1}{2}|\alpha|^2} \\ D(\alpha)D(\beta) = e^{\alpha a^\dagger - \alpha^* a} e^{\beta a^\dagger - \beta^* a} = D(\alpha+\beta) e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \\ D(\alpha)D(-\alpha) = 1 \\ e^{-(\alpha a^\dagger - \alpha^* a)} a e^{\alpha a^\dagger - \alpha^* a} = \exp(-\mathrm{ad}_{(\alpha a^\dagger - \alpha^* a)}) a = a + \alpha \\ e^{-(\alpha a^\dagger - \alpha^* a)} a^\dagger e^{\alpha a^\dagger - \alpha^* a} = \exp(-\mathrm{ad}_{(\alpha a^\dagger - \alpha^* a)}) a^\dagger = a^\dagger + \alpha^* \end{cases} . \tag{A.7}$$

- coherent states 满足

$$\begin{cases} \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2 \langle\alpha|\alpha\rangle \\ \langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0|D(\alpha)|0\rangle = \frac{\alpha^n}{\sqrt{n!}} e^{-\frac{1}{2}|\alpha|^2} \\ \langle\alpha|\beta\rangle = \langle 0|D(-\alpha)D(\beta)|0\rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\beta|^2 - 2\alpha^*\beta)} \end{cases} . \tag{A.8}$$

calculation:

注意

$$\begin{cases} [a, (a^\dagger)^n] = n(a^\dagger)^{n-1} \\ \langle 0|a^n (a^\dagger)^n|0\rangle = n! \end{cases} \Longrightarrow |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle, \tag{A.9}$$

那么

$$\langle n|\alpha\rangle = \langle n|e^{\alpha a^\dagger - \alpha^* a}|0\rangle = \frac{1}{\sqrt{n!}} \sum_{m=0}^{\infty} \frac{1}{m!} \langle 0|a^n (\alpha a^\dagger - \alpha^* a)^m|0\rangle, \tag{A.10}$$

其中

$$\begin{aligned} \langle 0|a^n(\alpha a^\dagger - \alpha^* a)^m|0\rangle &= m\alpha \langle 0|a^{n-1}(\alpha a^\dagger - \alpha^* a)^{m-1}|0\rangle \\ &= \begin{cases} 0 & m < n \\ \frac{m!\alpha^n}{(m-n)!} \langle 0|(\alpha a^\dagger - \alpha^* a)^{m-n}|0\rangle & m \geq n \end{cases}, \end{aligned} \tag{A.11}$$

代入, 得

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0|D(\alpha)|0\rangle, \tag{A.12}$$

其中

$$\langle 0|D(\alpha)|0\rangle = \langle 0|e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a}|0\rangle = e^{-\frac{1}{2}|\alpha|^2}. \tag{A.13}$$

- 因此

$$I = \frac{1}{\pi} \int d^2\alpha\ |\alpha\rangle\langle\alpha|, \quad d^2\alpha \equiv d\mathrm{Re}(\alpha) d\mathrm{Im}(\alpha). \tag{A.14}$$

proof:

考虑

$$\int d^2\alpha\ \langle m|\alpha\rangle\langle\alpha|n\rangle = \frac{1}{\sqrt{m!n!}} \int d^2\alpha\, \alpha^m (\alpha^*)^n e^{-|\alpha|^2}$$

$$
\begin{aligned}
&= \frac{1}{\sqrt{m!n!}} \int_0^\infty r dr \int_0^{2\pi} d\theta \, r^{m+n} e^{i(m-n)\theta} e^{-r^2} \\
&= \begin{cases} 0 & m \neq n \\ \dfrac{2\pi}{n!} \displaystyle\int_0^\infty dr \, r^{2n+1} e^{-r^2} & m = n \end{cases} = \pi \delta_{mn}.
\end{aligned} \tag{A.15}
$$

- $a^\dagger$ 没有 eigenket, 但有

$$
a^\dagger |\alpha\rangle \langle\alpha| = \left(\frac{\partial}{\partial\alpha} + \alpha^*\right) |\alpha\rangle \langle\alpha| . \tag{A.16}
$$

proof:

根据 (A.4), 有

$$
a^\dagger |\alpha\rangle \langle\alpha| = e^{\alpha a^\dagger - \alpha^* a} |1\rangle \langle\alpha| + \alpha^* |\alpha\rangle \langle\alpha| , \tag{A.17}
$$

并且

$$
\begin{aligned}
\frac{\partial}{\partial\alpha} |\alpha\rangle \langle\alpha| &= \frac{\partial}{\partial\alpha} \left(e^{\frac{1}{2}|\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger} |0\rangle \langle 0| e^{-\frac{1}{2}|\alpha|^2} e^{-\alpha a^\dagger} e^{\alpha^* a} \right) \\
&= D(\alpha) \left(\frac{1}{2}\alpha^* + a^\dagger \right) |0\rangle \langle\alpha| + |\alpha\rangle \langle 0| \left(-\frac{1}{2}\alpha^* - a^\dagger \right) D(-\alpha) \\
&= D(\alpha) |1\rangle \langle\alpha| - |\alpha\rangle \langle 1| D(-\alpha)
\end{aligned} \tag{A.18}
$$