

Numerical Path Integral

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1 path integral in quantum mechanics

- 考虑系统的 Hamiltonian 为

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

那么其 Lagrangian 为

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

系统初态为 $|\psi_0\rangle$.

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

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

其中 $\Delta t = \frac{T}{N+1}$.

- 数值计算中, 令

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

那么

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

1.1 Gaussian wave packet

- 考虑一个自由粒子, 初态为

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

那么, 预期结果为

$$\psi(t, x) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{m}{m+2it}} \exp\left(\frac{m}{m+2it}(-x^2 + ik_0 x) - i\frac{k_0^2}{2(m+2it)}t\right). \quad (1.7)$$

- 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):

```
1 psi_final = psi_0
2 for i in range(N+1):
3     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):

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

或

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

- 另外, 根据经验, 需要有 $|\Delta x \sqrt{\frac{m}{2\pi i \Delta t}}|^2 \ll 1$, 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):

$$L = 400, M = 24000, N = 10$$

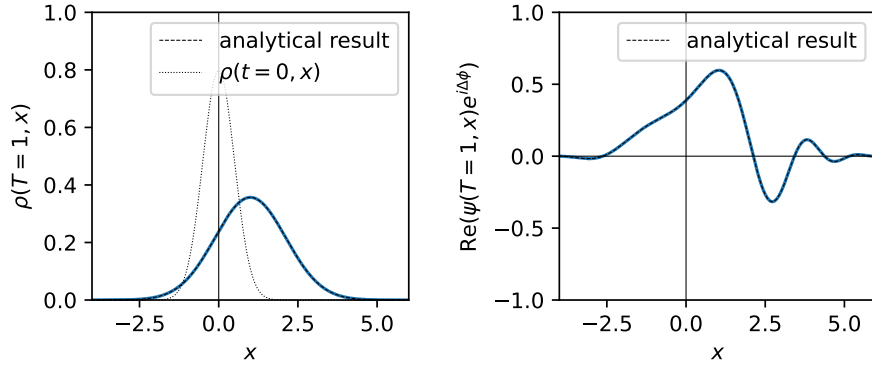


Figure 1: numerical path integral (normalized) at $T = 1$ with $A \sim 10^{18}, \Delta\phi \approx \pi + 0.7$.

1.2 harmonic oscillator and coherent states

- 考虑谐振子的 coherent states,

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

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

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

这对数值结果有微小的改进.

- 数值计算结果如下:

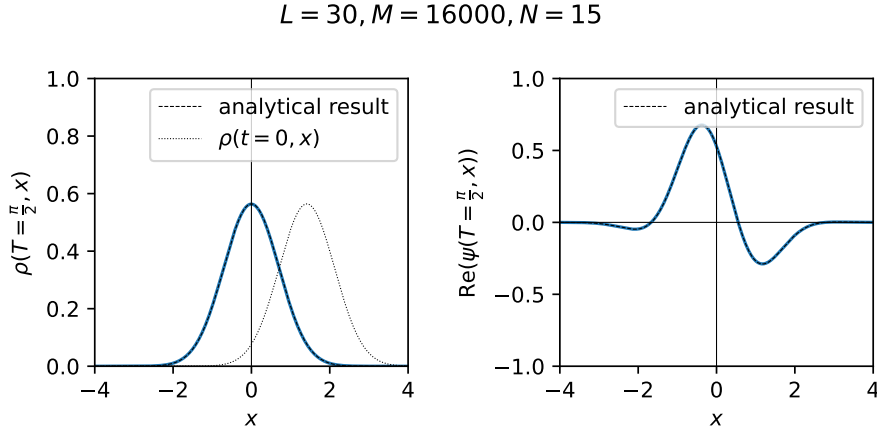


Figure 2: numerical path integral at $T = \frac{\pi}{2}$.

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 and displacement operators

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

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

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

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

calculation:

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

因此

$$\begin{cases} a |\alpha\rangle = \dots \\ a^\dagger |\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a} |1\rangle + \alpha^* |\alpha\rangle \\ a^\dagger a |\alpha\rangle = \alpha a^\dagger |\alpha\rangle \Rightarrow \langle \alpha | a^\dagger a | \alpha \rangle = |\alpha|^2 \langle \alpha | \alpha \rangle \end{cases}. \quad (A.4)$$

- displacement operator 是 unitary operator, 且满足

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

calculation:

首先

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

使用 BCH formula,

$$\begin{cases} e^A e^B = \exp \left(A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]] + \dots \right) \\ e^A B e^{-A} = e^{\text{ad}_A} B \\ e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\alpha a^\dagger - \alpha^* a + \frac{1}{2}|\alpha|^2} \\ D(\alpha)D(\beta) = e^{\alpha a^\dagger - \alpha^* a} e^{\beta a^\dagger - \beta^* a} = D(\alpha + \beta) e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \\ D(\alpha)D(-\alpha) = 1 \\ e^{-(\alpha a^\dagger - \alpha^* a)} a e^{\alpha a^\dagger - \alpha^* a} = \exp(-\text{ad}_{(\alpha a^\dagger - \alpha^* a)}) a = a + \alpha \\ e^{-(\alpha a^\dagger - \alpha^* a)} a^\dagger e^{\alpha a^\dagger - \alpha^* a} = \exp(-\text{ad}_{(\alpha a^\dagger - \alpha^* a)}) a^\dagger = a^\dagger + \alpha^* \end{cases} . \quad (\text{A.7})$$

- coherent states 满足

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

calculation:

注意

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

那么

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

其中

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

代入, 得

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

其中

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

- 因此

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

proof:

考虑

$$\begin{aligned} \int d^2\alpha \langle m|\alpha\rangle \langle \alpha|n\rangle &= \frac{1}{\sqrt{m!n!}} \int d^2\alpha \alpha^m (\alpha^*)^n e^{-|\alpha|^2} \\ &= \frac{1}{\sqrt{m!n!}} \int_0^\infty r dr \int_0^{2\pi} d\theta r^{m+n} e^{i(m-n)\theta} e^{-r^2} \\ &= \begin{cases} 0 & m \neq n \\ \frac{2\pi}{n!} \int_0^\infty dr r^{2n+1} e^{-r^2} & m = n \end{cases} = \pi \delta_{mn}. \end{aligned} \quad (\text{A.15})$$

- a^\dagger 没有 eigenket, 但有

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

proof:

根据 (A.4), 有

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

并且

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

B eigenstate of the field operator $\phi(\vec{x})$

- 首先需要找到 Hermitian operator

$$a + a^\dagger \quad (\text{B.1})$$

的 eigenstate.