

Numerical Path Integral

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Contents

1 path integral in quantum mechanics	1
1.1 Gaussian wave packet	1
1.2 harmonic oscillator and coherent states	2
A the coherent states	3

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
```

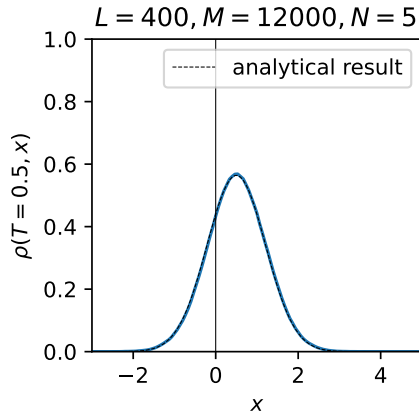
不推荐以下两种方法 (在 $T = 0.1, L = 300, M = 9000, N = 1$ 时可以得到较准确的波形):

```
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
```

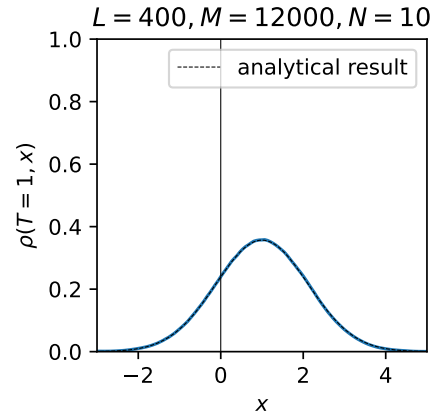
或

```
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):



(a) $T = 0.5$ and $A \sim 10^{11}$.



(b) $T = 1$ and $A \sim 10^{11}$.

Figure 1: numerical path integral.

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

$$\alpha = |\alpha| = 1 \quad (1.9)$$

的情况.

- 计算中可以让

$$K_{ij} = \sqrt{\frac{m}{2\pi i \Delta t}} \exp\left(i \frac{m}{2} \frac{(x_i - x_j)^2}{\Delta t}\right) \frac{e^{-i\Delta t V(x_i)} + e^{-i\Delta t V(x_j)}}{2}, \quad (1.10)$$

这对数值结果有微小的改进.

- 数值计算结果如下:

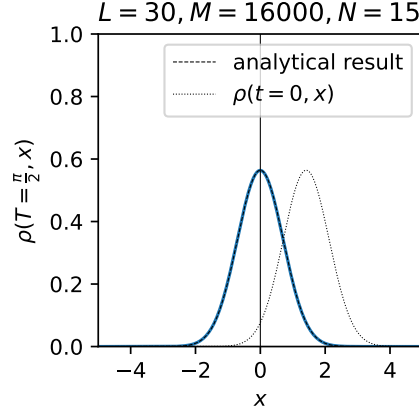


Figure 2: numerical path integral at $T = \frac{\pi}{2}$.

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

A the coherent states

- coherent states 是 annihilation operator 的本征态

$$\begin{cases} a |\alpha\rangle = \alpha |\alpha\rangle, \alpha \in \mathbb{C} \\ |\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a} |0\rangle \end{cases} \quad (A.1)$$

proof:

$$\begin{cases} [a, (\alpha a^\dagger - \alpha^* a)^n] = n\alpha(\alpha a^\dagger - \alpha^* a)^{n-1} \\ [a^\dagger, (\alpha a^\dagger - \alpha^* a)^n] = n\alpha^*(\alpha a^\dagger - \alpha^* a)^{n-1} \end{cases} \implies \begin{cases} [a, e^{\alpha a^\dagger - \alpha^* a}] = \alpha e^{\alpha a^\dagger - \alpha^* a} \\ [a^\dagger, e^{\alpha a^\dagger - \alpha^* a}] = \alpha^* e^{\alpha a^\dagger - \alpha^* a} \end{cases} \quad (A.2)$$

因此

$$\begin{cases} a |\alpha\rangle = \dots \\ a^\dagger |\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a} |1\rangle + \alpha^* |\alpha\rangle \end{cases} \quad (A.3)$$

- 并且

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

calculation:

content...