Numerical Path Integral

Siyang Wan (万思扬)

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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 $\Delta t = \frac{T}{N+1}$.

- 数值计算中, 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

$$\psi_0(x) = \Big(\frac{2}{\pi}\Big)^{\frac{1}{4}} e^{-x^2+ik_0x}, \quad \langle k|\psi_0\rangle = \frac{1}{(2\pi)^{1/4}}e^{-\frac{1}{4}(k-k_0)^2}, \tag{1.6}$$

  那么, 预期结果为

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

- 计算 (1.5) 最快 (且节省内存) 的方法是:

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

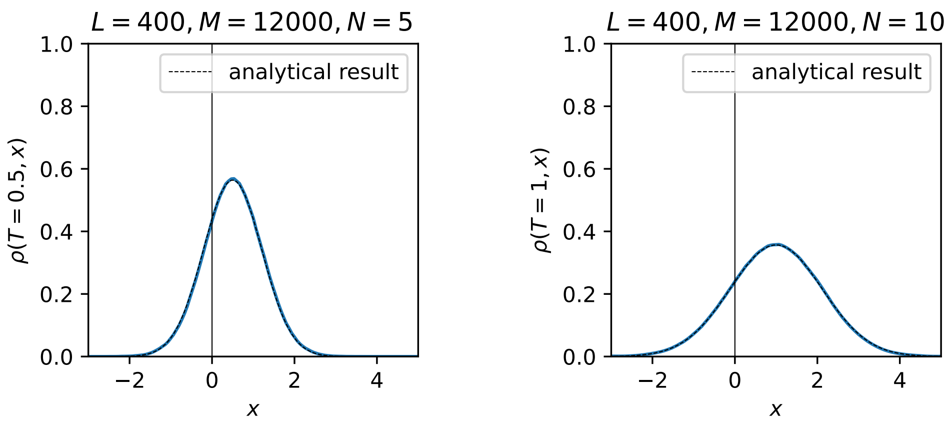
不推荐以下两种方法 (在 $T = 0.1, L = 300, M = 9000, N = 1$ 时可以得到较准确的波形):

```
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 $\sim 10^{-2}$.
- 用路径积分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) $T = 0.1$ and $A \sim 10^{11}$.

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

Figure 1: numerical path integral.