

Path Integral Numerically

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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:

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

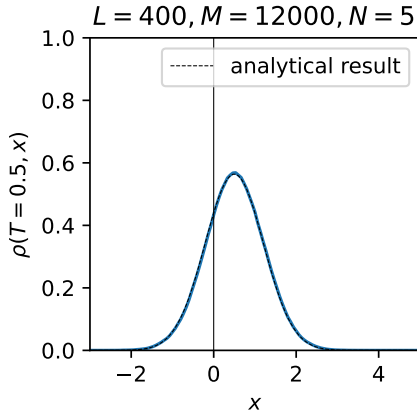
不推荐以下两种方法 (在 $T = 0.1, L = 300, M = 9000, N = 1$ 时可以得到较准确的波形):

```
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
```

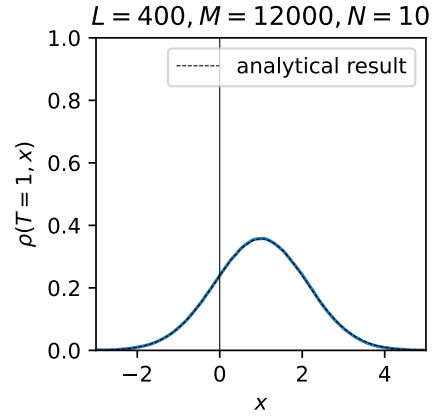
或

```
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 $\sim 10^{-2}$.
- 用路径积分数值计算得到的结果如下图所示 ($A = \int dx \rho$ 是 normalization constant):



(a) $T = 0.1$ and $A \sim 10^{11}$.



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

Figure 1: path integral numerically.