Path Integral Numerically

Siyang Wan (万思扬)

June 2, 2025

Contents

1 path integral **1**
1.1 Gaussian wave packet 1

1 path integral

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

- 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):

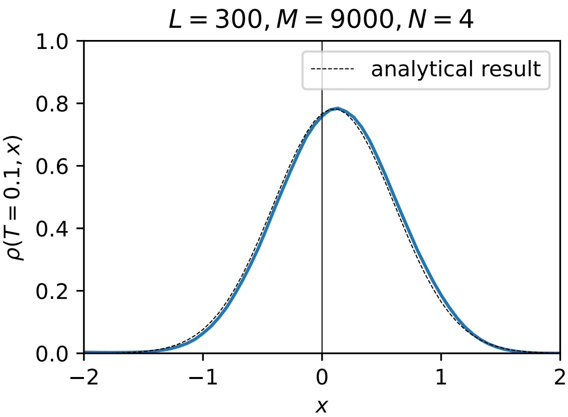

Figure 1: path integral numerically (normalized, $A \sim 10^{11}$) with $T = 0.1$.