Numerical Path Integral

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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

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

- 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):

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

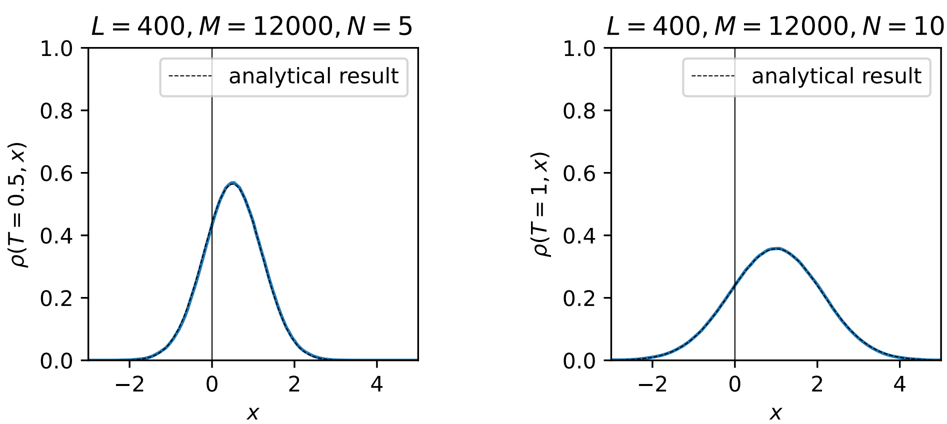
不推荐以下两种方法 (在 $T = 0.1, L = 300, M = 9000, N = 1$ 时可以得到较准确的波形):

```
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 $\sim 10^{-2}$.
- 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) $T = 0.1$ 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,

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

其中 $\alpha \in \mathbb{C}$.

- 令 $m = \omega = 1$, 考虑初始条件为

$$\alpha = |\alpha| = 1 \tag{1.9}$$

的情况.

- 计算中可以让

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

  这对数值结果有微小的改进.

- 数值计算结果如下:

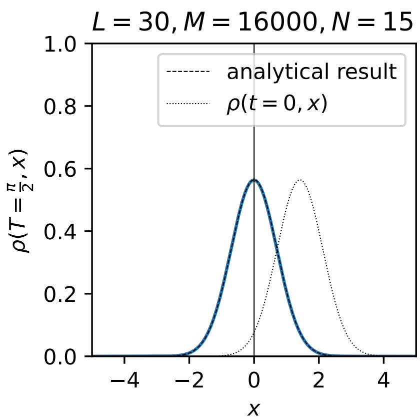


Figure 2: numerical path integral at $T = \frac{\pi}{2}$.

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

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

proof:

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

因此

$$\begin{cases} a\left|\alpha\right\rangle = \cdots \\ a^\dagger\left|\alpha\right\rangle = e^{\alpha a^\dagger - \alpha^* a}\left|1\right\rangle + \alpha^*\left|\alpha\right\rangle \end{cases}. \tag{A.3}$$

- 并且

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

calculation:

content...