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

- 数値计算中, 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

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

那么, 预期结果为

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

- 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):

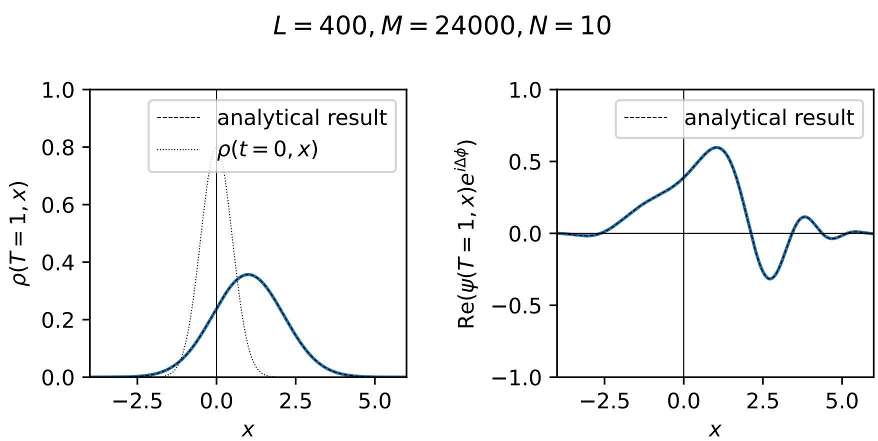

Figure 1: numerical path integral (normalized) at $T=1$ with $A\sim 10^{18}, \Delta\phi \approx \pi + 0.7$.

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 $\alpha=|\alpha|=1$ 的情况. 计算中可以让

$$K_{ij}=\sqrt{\frac{m}{2\pi i\Delta t}}\exp\left(i\frac{m}{2}\frac{(x_i-x_j)^2}{\Delta t}\right)\frac{e^{-i\Delta tV(x_i)}+e^{-i\Delta tV(x_j)}}{2}, \tag{1.9}$$

这对数值结果有微小的改进.

- 数值计算结果如下:

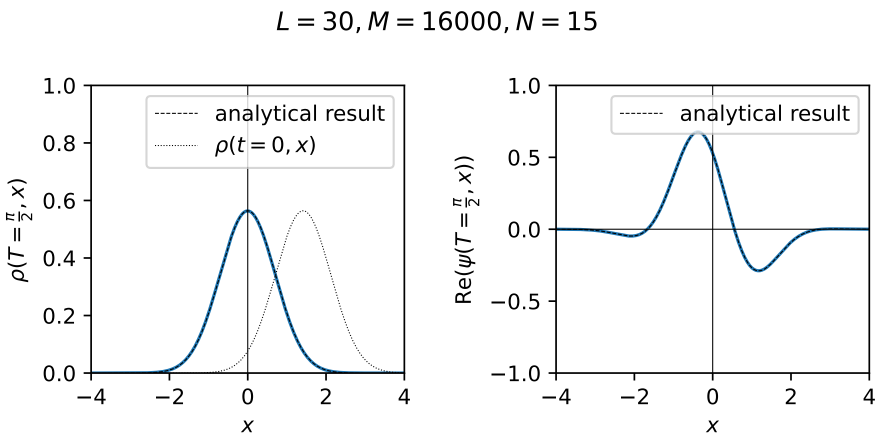

Figure 2: numerical path integral at $T=\frac{\pi}{2}$.

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

A coherent states and displacement operators

- 参考: Wikipedia: Coherent state, Wikipedia: Displacement operator.
- coherent states, $|\alpha\rangle$, 是 annihilation operator 的本征态

$$\begin{cases} a\,|\alpha\rangle=\alpha\,|\alpha\rangle\,,\alpha\in\mathbb{C} \\ |\alpha\rangle=D(\alpha)\,|0\rangle \end{cases}, \tag{A.1}$$

其中 $D(\alpha)$ 是 displacement operators,

$$D(\alpha):=e^{\alpha a^\dagger-\alpha^* a}. \tag{A.2}$$

calculation:

$$\begin{cases} [a,(\alpha a^\dagger-\alpha^* a)^n]=n\alpha(\alpha a^\dagger-\alpha^* a)^{n-1} \\ [a^\dagger,(\alpha a^\dagger-\alpha^* a)^n]=n\alpha^*(\alpha a^\dagger-\alpha^* a)^{n-1} \\ [a^\dagger a,(\alpha a^\dagger-\alpha^* a)^n]=n(\alpha a^\dagger+\alpha^* a)(\alpha a^\dagger-\alpha^* a)^{n-1}-n(n-1)|\alpha|^2(\alpha a^\dagger-\alpha^* a)^{n-2} \end{cases}$$
$$\Longrightarrow\begin{cases} [a,e^{\alpha a^\dagger-\alpha^* a}]=\alpha e^{\alpha a^\dagger-\alpha^* a} \\ [a^\dagger,e^{\alpha a^\dagger-\alpha^* a}]=\alpha^* e^{\alpha a^\dagger-\alpha^* a} \\ [a^\dagger a,e^{\alpha a^\dagger-\alpha^* a}]=(\alpha a^\dagger+\alpha^* a-|\alpha|^2)e^{\alpha a^\dagger-\alpha^* a} \end{cases}, \tag{A.3}$$

因此

$$\begin{cases} a\,|\alpha\rangle=\cdots \\ a^\dagger\,|\alpha\rangle=e^{\alpha a^\dagger-\alpha^* a}\,|1\rangle+\alpha^*\,|\alpha\rangle \\ a^\dagger a\,|\alpha\rangle=\alpha a^\dagger\,|\alpha\rangle\Longrightarrow\langle\alpha|a^\dagger a|\alpha\rangle=|\alpha|^2\,\langle\alpha|\alpha\rangle \end{cases}. \tag{A.4}$$

- displacement operator 是 unitary operator, 且满足

$$\begin{cases} D(\alpha) := e^{\alpha a^\dagger - \alpha^* a} = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\frac{1}{2}|\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger} \\ D(\alpha)D(\beta) = e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} D(\alpha+\beta) \\ D^\dagger(\alpha) = D(-\alpha) \\ D^\dagger(\alpha) a D(\alpha) = a + \alpha \\ D^\dagger(\alpha) a^\dagger D(\alpha) = a^\dagger + \alpha^* \end{cases} . \tag{A.5}$$

calculation:

首先

$$D^\dagger(\alpha) = \sum_{n=0}^{\infty} \frac{1}{n!}((\alpha a^\dagger - \alpha^* a)^\dagger)^n = \sum_{n=0}^{\infty} \frac{1}{n!}(\alpha^* a - \alpha a^\dagger)^n = D(-\alpha), \tag{A.6}$$

使用 BCH formula,

$$\begin{cases} e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] - \frac{1}{12}[B,[A,B]] + \cdots\right) \\ e^A B e^{-A} = e^{\mathrm{ad}_A} B \end{cases}$$

$$\Longrightarrow \begin{cases} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\alpha a^\dagger - \alpha^* a + \frac{1}{2}|\alpha|^2} \\ D(\alpha)D(\beta) = e^{\alpha a^\dagger - \alpha^* a} e^{\beta a^\dagger - \beta^* a} = D(\alpha+\beta) e^{\frac{1}{2}(\alpha\beta^* - \alpha^*\beta)} \\ D(\alpha)D(-\alpha) = 1 \\ e^{-(\alpha a^\dagger - \alpha^* a)} a e^{\alpha a^\dagger - \alpha^* a} = \exp(-\mathrm{ad}_{(\alpha a^\dagger - \alpha^* a)}) a = a + \alpha \\ e^{-(\alpha a^\dagger - \alpha^* a)} a^\dagger e^{\alpha a^\dagger - \alpha^* a} = \exp(-\mathrm{ad}_{(\alpha a^\dagger - \alpha^* a)}) a^\dagger = a^\dagger + \alpha^* \end{cases} . \tag{A.7}$$

- coherent states 满足

$$\begin{cases} \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2 \langle\alpha|\alpha\rangle \\ \langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0|D(\alpha)|0\rangle = \frac{\alpha^n}{\sqrt{n!}} e^{-\frac{1}{2}|\alpha|^2} \\ \langle\alpha|\beta\rangle = \langle 0|D(-\alpha)D(\beta)|0\rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\beta|^2 - 2\alpha^*\beta)} \end{cases} . \tag{A.8}$$

calculation:

注意

$$\begin{cases} [a, (a^\dagger)^n] = n(a^\dagger)^{n-1} \\ \langle 0|a^n (a^\dagger)^n|0\rangle = n! \end{cases} \Longrightarrow |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle , \tag{A.9}$$

那么

$$\langle n|\alpha\rangle = \langle n|e^{\alpha a^\dagger - \alpha^* a}|0\rangle = \frac{1}{\sqrt{n!}} \sum_{m=0}^{\infty} \frac{1}{m!} \langle 0|a^n (\alpha a^\dagger - \alpha^* a)^m|0\rangle , \tag{A.10}$$

其中

$$\begin{aligned} \langle 0|a^n (\alpha a^\dagger - \alpha^* a)^m|0\rangle &= m\alpha \langle 0|a^{n-1} (\alpha a^\dagger - \alpha^* a)^{m-1}|0\rangle \\ &= \begin{cases} 0 & m < n \\ \frac{m!\alpha^n}{(m-n)!} \langle 0|(\alpha a^\dagger - \alpha^* a)^{m-n}|0\rangle & m \geq n \end{cases} , \end{aligned} \tag{A.11}$$

代入, 得

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0|D(\alpha)|0\rangle , \tag{A.12}$$

其中

$$\langle 0|D(\alpha)|0\rangle = \langle 0|e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a}|0\rangle = e^{-\frac{1}{2}|\alpha|^2}. \tag{A.13}$$

- 因此
$$I = \frac{1}{\pi}\int d^2\alpha \, |\alpha\rangle\langle\alpha|, \quad d^2\alpha \equiv d\mathrm{Re}(\alpha)d\mathrm{Im}(\alpha). \tag{A.14}$$

proof:

考虑

$$\begin{aligned}\int d^2\alpha \, \langle m|\alpha\rangle\langle\alpha|n\rangle &= \frac{1}{\sqrt{m!n!}}\int d^2\alpha \, \alpha^m(\alpha^*)^n e^{-|\alpha|^2} \\ &= \frac{1}{\sqrt{m!n!}}\int_0^\infty rdr\int_0^{2\pi} d\theta \, r^{m+n}e^{i(m-n)\theta}e^{-r^2} \\ &= \begin{cases} 0 & m\neq n \\ \dfrac{2\pi}{n!}\displaystyle\int_0^\infty dr\, r^{2n+1}e^{-r^2} & m=n \end{cases} = \pi\delta_{mn}. \end{aligned}\tag{A.15}$$

- $a^\dagger$ 没有 eigenket, 但有
$$a^\dagger|\alpha\rangle\langle\alpha| = \left(\frac{\partial}{\partial\alpha}+\alpha^*\right)|\alpha\rangle\langle\alpha|. \tag{A.16}$$

proof:

根据 (A.4), 有

$$a^\dagger|\alpha\rangle\langle\alpha| = e^{\alpha a^\dagger-\alpha^* a}|1\rangle\langle\alpha| + \alpha^*|\alpha\rangle\langle\alpha|, \tag{A.17}$$

并且

$$\begin{aligned}\frac{\partial}{\partial\alpha}|\alpha\rangle\langle\alpha| &= \frac{\partial}{\partial\alpha}\left(e^{\frac{1}{2}|\alpha|^2}e^{-\alpha^* a}e^{\alpha a^\dagger}|0\rangle\langle 0|e^{-\frac{1}{2}|\alpha|^2}e^{-\alpha a^\dagger}e^{\alpha^* a}\right) \\ &= D(\alpha)\left(\frac{1}{2}\alpha^*+a^\dagger\right)|0\rangle\langle\alpha| + |\alpha\rangle\langle 0|\left(-\frac{1}{2}\alpha^*-a^\dagger\right)D(-\alpha) \\ &= D(\alpha)|1\rangle\langle\alpha|. \end{aligned}\tag{A.18}$$

B simultaneous eigenstates of the field operators $\phi(\vec{x})$

- 场算符可以写作
$$\phi(\vec{x}) = \int\frac{d^Dk}{(2\pi)^{D/2}\sqrt{2\omega_k}}(a_{\vec{k}}e^{i\vec{k}\cdot\vec{x}} + a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{x}}), \tag{B.1}$$
并注意到
$$\begin{cases}[\phi(\vec{x}),\phi(\vec{y})]=0 \\ [(a_{\vec{k}_1}e^{i\vec{k}_1\cdot\vec{x}}+a_{\vec{k}_1}^\dagger e^{-i\vec{k}_1\cdot\vec{x}}),(a_{\vec{k}_2}e^{i\vec{k}_2\cdot\vec{y}}+a_{\vec{k}}^\dagger e^{-i\vec{k}_2\cdot\vec{y}})] = i\delta^{(D)}(\vec{k}_1-\vec{k}_2)\sin(\vec{k}_1\cdot(\vec{x}-\vec{y}))\end{cases}, \tag{B.2}$$
可见:
  1. $\phi(\vec{x}), \forall\vec{x}$ 有共同本征态,
  2. $\phi(\vec{x})$ 和 $(a_{\vec{k}}e^{i\vec{k}\cdot\vec{x}}+a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{x}}), \forall\vec{k}$ 有共同本征态,
  3. $\phi(\vec{y})$ 和 $(a_{\vec{k}}e^{i\vec{k}\cdot\vec{x}}+a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{x}}), \vec{x}\neq\vec{y}$ 不具有共同本征态.
- 引入平移算符
$$U(\vec{x}) = e^{-i\vec{P}\cdot\vec{x}}, \quad \vec{P} = \int d^Dk\,\vec{k}a_{\vec{k}}^\dagger a_{\vec{k}}, \tag{B.3}$$
那么
$$\phi(\vec{x}) = U(\vec{x})\phi(0)U^\dagger(\vec{x}). \tag{B.4}$$
- 因此, 只需要先找到 $\phi(0)$ 的本征态, 并对其线性组合使得
$$\begin{cases}\phi(0)|\lambda\rangle = \lambda(0)|\lambda\rangle \\ U(\vec{x})|\lambda\rangle = |\lambda\rangle\end{cases}, \tag{B.5}$$
就得到所有场算符的共同本征态.

B.1 eigenstates of $\phi(0)$

- 令

$$\begin{cases} p_{\vec{k}} = \dfrac{a_{\vec{k}} - a^\dagger_{\vec{k}}}{\sqrt{2}i} \\ q_{\vec{k}} = \dfrac{a_{\vec{k}} + a^\dagger_{\vec{k}}}{\sqrt{2}} \end{cases}, \tag{B.6}$$

那么

$$\phi(0) = \int \frac{d^D k}{(2\pi)^{D/2}\sqrt{\omega_k}} q_{\vec{k}}. \tag{B.7}$$

- 注意到

$$\begin{cases} [q_{\vec{k}_1}, p_{\vec{k}_2}] = i\delta^{(D)}(\vec{k}_1 - \vec{k}_2) \\ a^\dagger_{\vec{k}} a_{\vec{k}} + \dfrac{1}{2}\delta^{(D)}(0) = \dfrac{1}{2}(p^2_{\vec{k}} + q^2_{\vec{k}}) \end{cases}. \tag{B.8}$$

- 令

$$|q_{\vec{k}}\rangle \in \mathrm{span}(|n_{\vec{k}}\rangle, n_{\vec{k}} = 0, 1, \cdots), \tag{B.9}$$

那么 (一维谐振子 $m\omega = 1/\delta^{(D)}(0)$)

$$\psi_{n_{\vec{k}}}(q_{\vec{k}}) = \langle q_{\vec{k}} | n_{\vec{k}}\rangle = \left(\frac{\delta^{(D)}(0)}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^{n_{\vec{k}}} n_{\vec{k}}!}} H_{n_{\vec{k}}}(\sqrt{\delta^{(D)}(0)} q_{\vec{k}}) e^{-\frac{\delta^{(D)}(0) q^2_{\vec{k}}}{2}}, \tag{B.10}$$

因此

$$\langle q_{\vec{k}} | 0\rangle = \delta(\vec{q}_{\vec{k}}) \tag{B.11}$$

C eigenstates of the field operators $\phi(\vec{x})$

- 场算符可以表示为

$$\phi(\vec{x}) = \int \frac{d^D k}{(2\pi)^{D/2}\sqrt{2\omega_k}} (a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + a^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}), \tag{C.1}$$

并且 $[\phi(\vec{x}), \phi(\vec{y})] = 0$.

- 首先需要找到 Hermitian operator

$$a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + a^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \tag{C.2}$$

的 eigenstate.

- 令

$$\begin{cases} p_{\vec{k}} = \dfrac{a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} - a^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}}{\sqrt{2}i} \\ q_{\vec{k}} = \dfrac{a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + a^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}}{\sqrt{2}} \end{cases}, \quad a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2} = \frac{1}{2}(p^2_{\vec{k}} + q^2_{\vec{k}}), \tag{C.3}$$

因此, $\phi(\vec{x})$ 可以写作

$$\begin{cases} \phi(\vec{x}) = \displaystyle\int \frac{d^D k}{(2\pi)^{D/2}\sqrt{\omega_k}} q_{\vec{k}} \\ [q_{\vec{k}_1}, q_{\vec{k}_2}] = i\delta^{(D)}(\vec{k}_1 - \vec{k}_2) \sin((\vec{k}_1 - \vec{k}_2)\cdot\vec{x}) = 0 \end{cases}, \tag{C.4}$$

$q_{\vec{k}}$ 的本征态为

$$\begin{cases} \hat{q}_{\vec{k}} |q_{\vec{k}}\rangle = q_{\vec{k}} |q_{\vec{k}}\rangle \\ e^{-in_{\vec{k}}\vec{k}\cdot\vec{x}} \langle n_{\vec{k}} | q_{\vec{k}}\rangle = \psi^*_{n_{\vec{k}}}(q_{\vec{k}}) \end{cases}, \quad q_{\vec{k}} \in \mathbb{R}, \tag{C.5}$$

其中

$$\begin{cases} |n_{\vec{k}}\rangle = \dfrac{(a^\dagger_{\vec{k}})^n}{\sqrt{n_{\vec{k}}!}} |0\rangle \\ \psi_n(q) = \psi^*_n(q) = \dfrac{1}{\pi^{1/4}\sqrt{2^n n!}} H_n(q) e^{-\frac{q^2}{2}} \\ H_n(q) = (-1)^n e^{q^2} \dfrac{d^n}{dq^n} e^{-q^2} \end{cases}. \tag{C.6}$$

remark:

注意到

$$\begin{aligned}\langle p|n\rangle &= \frac{1}{\sqrt{2\pi}}\tilde{\psi}_n(p) = \int dq\,\frac{e^{-ipq}}{\sqrt{2\pi}}\psi_n(q)\\ &= \frac{1}{\pi^{1/4}\sqrt{2^n n!}}\frac{1}{\sqrt{2\pi}}\int dq\, e^{-ipq-\frac{q^2}{2}}H_n(q),\end{aligned} \tag{C.7}$$

其中

$$\int dq\, e^{-ipq-\frac{q^2}{2}}H_n(q) = (-i)^n\sqrt{2\pi}H_n(p)e^{-\frac{p^2}{2}}, \tag{C.8}$$

因此

$$\langle p|n\rangle = \frac{1}{\sqrt{2\pi}}\tilde{\psi}_n(p) = (-i)^n\frac{1}{\pi^{1/4}\sqrt{2^n n!}}H_n(p)e^{-\frac{p^2}{2}} = (-i)^n\psi_n(p). \tag{C.9}$$

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proof of (C.8):
用 Hermitian polynomials 的 generating function (参考 Wikipedia: Hermitian polynomials)

$$e^{2xt-t^2} = \sum_{n=0}^{\infty}\frac{H_n(x)}{n!}t^n, \tag{C.10}$$

有

$$\int dq\, e^{-ipq-\frac{q^2}{2}+(2qt-t^2)} = \sqrt{2\pi}e^{-2ipt+t^2}e^{-\frac{p^2}{2}} = \sqrt{2\pi}e^{-\frac{p^2}{2}}\sum_{n=0}^{\infty}\frac{H_n(p)}{n!}(-it)^n. \tag{C.11}$$