《量子信息基础》：

1. (1) Construct the full analytic equations for the normalized wave functions ψ_2 and ψ_3 of harmonic oscillators. (ψ_0 and ψ_1 are done in example 2.4 in the text book*)

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)$$

$$\begin{aligned}
\psi_1 = a_+\psi_0 &= \frac{1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[-\hbar\left(-\frac{m\omega}{2\hbar}\right)2x + m\omega x\right] exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2m\omega x exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} x exp\left(-\frac{m\omega}{2\hbar}x^2\right)
\end{aligned}$$

$$\begin{aligned}
\psi_2 = \frac{1}{\sqrt{2}}(a_+)^2\psi_0 &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2m\omega x exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{2}}\frac{1}{\hbar}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(-\hbar\frac{d}{dx} + m\omega x\right) x exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{2}}\frac{1}{\hbar}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(-\hbar\left(1 - x\frac{m\omega}{2\hbar}2x\right) + m\omega x^2\right) exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2 - 1\right) exp\left(-\frac{m\omega}{2\hbar}x^2\right)
\end{aligned}$$

$$\begin{aligned}
\psi_3 = \frac{1}{\sqrt{6}}(a_+)^3\psi_0 &= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\frac{2m\omega}{\hbar}x^2 - 1\right) exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{2m\omega}{\hbar}\left(-\hbar\frac{d}{dx} + m\omega x\right) x^2 exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&- \frac{1}{\sqrt{6}}\frac{1}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(-\hbar\frac{d}{dx} + m\omega x\right) exp\left(-\frac{m\omega}{2\hbar}x^2\right) = \\
&= \frac{1}{\sqrt{3}}\frac{1}{\sqrt{\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{m\omega}{\hbar}(-2x\hbar + 2m\omega x^3) exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&- \frac{1}{\sqrt{3}}\frac{1}{\sqrt{\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}(m\omega x) exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
&= \frac{1}{\sqrt{3}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(\frac{m\omega}{\hbar}\right)^{1/2}\left(-3x + \frac{2m\omega x^3}{\hbar}\right) exp\left(-\frac{m\omega}{2\hbar}x^2\right)
\end{aligned}$$

(2) Prove the orthonormality of the stationary states of the harmonic oscillators (textbook* page 64).

$$\int_{-\infty}^{\infty}\psi_m^*\psi_n dx = \delta_{mn}$$

$$\int_{-\infty}^{\infty}\psi_m^*\,(a_+a_-)\psi_n dx = n\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = \int_{-\infty}^{\infty}(a_-\psi_m)^*\,(a_-\psi_n)dx$$
$$= \int_{-\infty}^{\infty}(a_+a_-\psi_m)^*\,\psi_n dx = m\int_{-\infty}^{\infty}\psi_m\,\psi_n dx$$

Unless $m = n$, $\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx$ must be zero. Due to normalization condition

$$\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = \delta_{mn}$$

2. <即教材*问题 2.12 和 Example 2.5>
   Starting from equation 2.69, find $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$, and $\langle T\rangle$ for the *n*-th stationary state of the harmonic oscillator. Check the uncertainty principle between $\langle x\rangle$ and $\langle p\rangle$ is satisfied.

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-), \qquad p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-)$$
$$a_+\psi_n = \sqrt{n+1}\psi_{n+1}, \qquad a_-\psi_n = \sqrt{n}\psi_{n-1}$$

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\int \psi_n^*(a_+ + a_-)\psi_n dx$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\int \psi_n^*\psi_{n+1}dx + \sqrt{n}\int \psi_n^*\psi_{n-1}dx\right] = 0$$

$$\langle p\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\int \psi_n^*(a_+ - a_-)\psi_n dx$$
$$= i\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n+1}\int \psi_n^*\psi_{n+1}dx - \sqrt{n}\int \psi_n^*\psi_{n-1}dx\right] = 0$$

$$x^2 = \frac{\hbar}{2m\omega}(a_+ + a_-)^2 = \frac{\hbar}{2m\omega}(a_+^2 + a_+a_- + a_-a_+ + a_-^2)^2$$
$$\begin{cases} a_+^2\psi_n = a_+\left(\sqrt{n+1}\psi_{n+1}\right) = \sqrt{n+1}\sqrt{n+2}\psi_{n+2} \\ a_+a_-\psi_n = a_+\left(\sqrt{n}\psi_{n-1}\right) = n\psi_n \\ a_-a_+\psi_n = a_-\left(\sqrt{n+1}\psi_{n+1}\right) = (n+1)\psi_n \\ a_-^2\psi_n = a_-\left(\sqrt{n}\psi_{n-1}\right) = \sqrt{n}\sqrt{n-1}\psi_{n-2} \end{cases}$$
$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\left[0 + n\int |\psi_n|^2 dx + (n+1)\int |\psi_n|^2 dx + 0\right] = \frac{\hbar}{2m\omega}(2n+1)$$
$$= \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega}$$

$$p^2 = -\frac{\hbar m\omega}{2}(a_+ - a_-)^2 = -\frac{\hbar m\omega}{2}(a_+^2 - a_+a_- - a_-a_+ + a_-^2)^2$$

$$\langle p^2\rangle = -\frac{\hbar m\omega}{2}\left[0 - n\int|\psi_n|^2dx - (n+1)\int|\psi_n|^2dx + 0\right] = \frac{\hbar m\omega}{2}(2n+1)$$
$$= \left(n+\frac{1}{2}\right)\hbar m\omega$$

$$\langle T\rangle = \langle\frac{p^2}{2m}\rangle = \left(n+\frac{1}{2}\right)\frac{\hbar\omega}{2}$$
$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{n+\frac{1}{2}}\sqrt{\frac{\hbar}{m\omega}},\quad \sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{n+\frac{1}{2}}\sqrt{\hbar m\omega}$$
$$\sigma_x\sigma_p = \left(n+\frac{1}{2}\right)\hbar \geq \frac{\hbar}{2}$$

3. (1) Prove that in the infinite square well, the wave function ψ_n satisfy the orthogonal condition

$$\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = \delta_{mn}$$

and write down the expansion formula for an arbitrary function *f*(*x*) (text book* Page 51).

$$\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx$$
$$= \frac{2}{a}\int_0^a \cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)dx$$
$$= \left\{\frac{1}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right\}\Big|_0^a$$
$$= \frac{1}{\pi}\left\{\frac{\sin((m-n)\pi)}{(m-n)} - \frac{\sin((m+n)\pi)}{(m+n)}\right\}$$

If m=n, $\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = 1$

If m≠n, $\int_{-\infty}^{\infty}\psi_m^*\,\psi_n dx = 0$

(2) <text book* Problem 2.37>

A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = A\sin^3(\pi x/a) \qquad (0 \leq x \leq a).$$

Determine *A*, find $\Psi(x,t)$, and calculate $\langle x\rangle$, as a function of time.

Hint: $\sin^n\theta$ and $\cos^n\theta$ can be reduced, by repeated application of the trigonometric sum formulas, to linear combinations of $\sin(m\theta)$ and $\cos(m\theta)$, with $m = 0, 1, 2, \ldots, n$.

$$\sin 3\theta = \sin\theta\cos 2\theta + \sin 2\theta\cos\theta = \sin\theta\,(1-2\sin^2\theta) + 2\sin\theta\,(1-\sin^2\theta)$$
$$= 3\sin\theta - 4\sin^3\theta$$
$$\psi_n(x) = \sqrt{\frac{a}{2}}\sin\left(\frac{n\pi x}{a}\right)$$
$$\Psi(x,0) = A\sin^3\left(\frac{\pi x}{a}\right) = A\left[\frac{3}{4}\sin\left(\frac{\pi x}{a}\right) - \frac{1}{4}\sin\left(\frac{3\pi x}{a}\right)\right]$$
$$= A\sqrt{\frac{a}{2}}\left[\frac{3}{4}\psi_1(x) - \frac{1}{4}\psi_3(x)\right]$$

$$\int_0^a |\Psi(x,0)|^2 dx = |A|^2 \frac{a}{2}\int_0^a \left|\frac{3}{4}\psi_1(x) - \frac{1}{4}\psi_3(x)\right|^2 dx = |A|^2 \frac{a}{2}\left(\frac{9}{16} - \frac{1}{16}\right) = 1$$

$$\therefore A = \sqrt{\frac{16}{5a}}$$

$$\Psi(x,0) = \frac{1}{\sqrt{10}}[3\psi_1(x) - \psi_3(x)]$$

$$\Psi(x,t) = \frac{1}{\sqrt{10}}\left[3\psi_1(x)e^{-iE_1 t/\hbar} - \psi_3(x)e^{-iE_3 t/\hbar}\right]$$

其中 $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

$$\langle x \rangle = \int_0^a x|\Psi(x,t)|^2 dx = \frac{9}{10}\int_0^a x\,\psi_1^2 dx + \frac{1}{10}\int_0^a x\,\psi_3^2 dx - \frac{3}{5}\cos(\omega t)\int_0^a x\,\psi_1\psi_3 dx$$

$$= \frac{9}{10}\langle x \rangle_1 + \frac{1}{10}\langle x \rangle_3 - \frac{3}{5}\cos(\omega t)\int_0^a x\,\psi_1\psi_3 dx$$

$$\langle x \rangle_n = \int_0^a x|\psi_n(x)|^2 dx = \frac{a}{2}$$

$$\int_0^a x\,\psi_1\psi_3 dx = \frac{2}{a}\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)dx$$

$$= \frac{2}{a}\int_0^a x\left[\cos\left(\frac{2\pi x}{a}\right) - \cos\left(\frac{4\pi x}{a}\right)\right]dx = 0$$

$$\therefore\ \langle x \rangle = \frac{9}{10}\frac{a}{2} + \frac{1}{10}\frac{a}{2} - 0 = \frac{a}{2}$$

4. Prove that for wave functions ψ, ϕ and operator A, the following two conditions hold.

$$\langle \psi|\phi\rangle = \langle \phi|\psi\rangle^*$$

$$|\psi\rangle = \begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\\ \cdots\\ \psi_N\end{bmatrix}$$

$$\langle \psi| = [\psi_1^* \quad \psi_2^* \quad \psi_3^* \quad \psi_4^* \quad \dots \quad \psi_N^*]$$

$$|\varphi\rangle = \begin{bmatrix}\varphi_1\\ \varphi_2\\ \varphi_3\\ \varphi_4\\ \cdots\\ \varphi_N\end{bmatrix}$$

$$\langle \varphi| = [\varphi_1^* \quad \varphi_2^* \quad \varphi_3^* \quad \varphi_4^* \quad \dots \quad \varphi_N^*]$$

$$\langle \psi|\phi\rangle = \psi_1^*\varphi_1 + \psi_2^*\varphi_2 + \psi_3^*\varphi_3 + \cdots + \psi_N^*\varphi_N$$
$$= (\varphi_1^*\psi_1 + \varphi_2^*\psi_2 + \varphi_3^*\psi_3 + \cdots + \varphi_N^*\psi_N)^* = \langle \phi|\psi\rangle^*$$

$$\langle \psi|A|\phi\rangle = \langle \phi|A^\dagger|\psi\rangle^*$$

由上式可得

$$\langle\psi|A\phi\rangle = \langle A\phi|\psi\rangle^* = \langle\phi|A^\dagger|\psi\rangle^*$$

或者用下面这个思路证明也可以：

$$\langle\psi|A|\phi\rangle = \int \psi^* A\,\phi dx = \int (\phi^* A^\dagger \psi)^* dx = \langle\phi|A^\dagger|\psi\rangle^*$$

5. (Ref to text book* Problem 3.39)
Find the matrix elements $\langle n|x|n'\rangle$ and $\langle n|p|n'\rangle$ in the orthonormal basis of stationary states for the harmonic oscillator $|n\rangle \equiv \psi_n(x)$. Construct the corresponding matrix a_+ and a_-, and construct the corresponding matrix $\hat{n}$ from the matrix a_+ and a_-.

$$a_+|n\rangle = \sqrt{n+1}|n+1\rangle$$
$$a_-|n\rangle = \sqrt{n}|n-1\rangle$$
$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-)$$
$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-)$$

$$\langle n|x|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|(a_+ + a_-)|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|a_+|n'\rangle + \sqrt{\frac{\hbar}{2m\omega}}\langle n|a_-|n'\rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta(n,n'+1) + \sqrt{n'}\delta(n,n'-1)\right)$$

或者写成：$\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta(n,n'+1) + \sqrt{n'}\delta(n,n'-1)\right)$ 也可以的。因为$n'+1=n$, delta 函数才等于 1

$$\langle n|p|n'\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\langle n|(a_+ - a_-)|n'\rangle = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\langle n|a_+|n'\rangle - i\sqrt{\frac{\hbar m\omega}{2}}\langle n|a_-|n'\rangle$$
$$= i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n}\delta(n,n'+1) - \sqrt{n'}\delta(n,n'-1)\right)$$

$$X = \sqrt{\frac{\hbar}{2m\omega}}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \\ 1 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \cdots & & & \end{bmatrix}$$

$$P = i\sqrt{\frac{\hbar m\omega}{2}}\begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \\ 1 & 0 & -\sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \cdots & & & \end{bmatrix}$$

$$A_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-iP + m\omega X) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \\ 1 & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \cdots & & & \end{bmatrix}$$

$$A_- = \frac{1}{\sqrt{2\hbar m\omega}}(iP + m\omega X) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \cdots & & & \end{bmatrix}$$

$$\hat{n} = A_+A_- = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \\ 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3 & 0 & \\ 0 & 0 & 0 & 0 & 4 & \\ & & \cdots & & & \end{bmatrix}$$

* David J. Griffiths, and Darrell F. Schroeter, Introduction to Quantum Mechanics (3rd Edition), Cambridge University Press (2018).