《量子信息基础》2024.3.21 随堂作业：

（2024.3.24 晚 22 点前提交）

1. (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).

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_m^* \psi_n dx &= \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx \\ &= \frac{1}{a}\int_0^a \cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)dx \\ &= \left\{\frac{1}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right\}\Bigg|_0^a \\ &= \frac{1}{\pi}\left\{\frac{\sin\big((m-n)\pi\big)}{(m-n)} - \frac{\sin\big((m+n)\pi\big)}{(m+n)}\right\}\end{aligned}$$

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

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

推导出正确结果给 10 分，只有推导或者只有结果给 5 分

(2) <text book* Problem 2.37>

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

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

Determine A, find $\Psi(x,t)$, and calculate $\langle x\rangle$, as a function of time. What is the expectation value of the energy? *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 $m = 0, 1, 2, \ldots, n$.

$$\begin{aligned}\sin 3\theta &= \sin\theta\cos 2\theta + \sin 2\theta\cos\theta = \sin\theta\,(1-2\sin^2\theta) + 2\sin\theta\,(1-\sin^2\theta) \\ &= 3\sin\theta - 4\sin^3\theta\end{aligned}$$

$$\psi_n(x) = \sqrt{\frac{a}{2}}\sin\left(\frac{n\pi x}{a}\right)$$ 系数应该是sqrt(2/a)

$$\begin{aligned}\Psi(x,0) = A\sin^3\left(\frac{\pi x}{a}\right) &= A\left[\frac{3}{4}\sin\left(\frac{\pi x}{a}\right) - \frac{1}{4}\sin\left(\frac{3\pi x}{a}\right)\right] \\ &= A\sqrt{\frac{a}{2}}\left[\frac{3}{4}\psi_1(x) - \frac{1}{4}\psi_3(x)\right]\end{aligned}$$

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

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

推导出 A 的正确结果给 10 分，只有推导或者只有结果给 5 分

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

$$\Psi(x,t)=\frac{1}{\sqrt{10}}\left[3\psi_1(x)e^{-iE_1t/\hbar}-\psi_3(x)e^{-iE_3t/\hbar}\right]$$

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

推导出$\Psi(x,t)$的正确结果给 10 分，只有推导或者只有结果给 5 分

$$\langle x\rangle=\int_0^a x|\Psi(x,t)|^2dx=\frac{9}{10}\int_0^a x\,\psi_1^2dx+\frac{1}{10}\int_0^a x\,\psi_3^2dx-\frac{3}{5}\cos(\omega t)\int_0^a x\,\psi_1\psi_3dx$$
$$=\frac{9}{10}\langle x\rangle_1+\frac{1}{10}\langle x\rangle_3-\frac{3}{5}\cos(\omega t)\int_0^a x\,\psi_1\psi_3dx$$

$$\langle x\rangle_n=\int_0^a x|\psi_n(x)|^2dx=\frac{a}{2}$$
$$\int_0^a x\,\psi_1\psi_3dx=\frac{2}{a}\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)dx$$
$$=\frac{1}{a}\int_0^a x\left[\cos\left(\frac{2\pi x}{a}\right)-\cos\left(\frac{4\pi x}{a}\right)\right]dx=0$$
$$\therefore\ \langle x\rangle=\frac{9}{10}\frac{a}{2}+\frac{1}{10}\frac{a}{2}-0=\frac{a}{2}$$

推导出$\langle x\rangle$的正确结果给 10 分，只有推导或者只有结果给 5 分

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

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

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

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

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

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

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

给出证明过程正确给 10 分，只有部分推导给 5 分

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

由上式可得

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

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

给出证明过程正确给 10 分，只有部分推导给 5 分

3. <即教材*问题 1.15>

Show that

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = 0$$

for any two (normalizable) solutions to the Schrödinger equation (with the same $\mathrm{V}(x)$), Ψ_1 and Ψ_2.

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = \int_{-\infty}^{\infty}\frac{\partial\Psi_1^*}{\partial t}\Psi_2 + \Psi_1^*\frac{\partial\Psi_2}{\partial \mathrm{t}}dx$$

推导到这步给 5 分

$$-i\hbar\frac{\partial\Psi_1^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1^*}{\partial x^2} + V\Psi_1^*$$

$$i\hbar\frac{\partial\Psi_2}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2}{\partial x^2} + V\Psi_2$$

给出正确的复共轭函数薛定谔方程给 10 分

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = \int_{-\infty}^{\infty}\left[\frac{\hbar}{2im}\frac{\partial^2\Psi_1^*}{\partial x^2} - \frac{V}{i\hbar}\Psi_1^*\right]\Psi_2 + \Psi_1^*\left[-\frac{\hbar}{2im}\frac{\partial^2\Psi_2}{\partial x^2} + \frac{V}{i\hbar}\Psi_2\right]dx$$

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = \int_{-\infty}^{\infty}\frac{\hbar}{2im}\frac{\partial^2\Psi_1^*}{\partial x^2}\Psi_2 - \Psi_1^*\frac{\hbar}{2im}\frac{\partial^2\Psi_2}{\partial x^2}dx$$

推导到这步给 5 分

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = \frac{\hbar}{2im}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\frac{\partial\Psi_1^*}{\partial x}\Psi_2 - \Psi_1^*\frac{\partial\Psi_2}{\partial x}\right)dx$$

推导到这步给 5 分

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = \frac{\hbar}{2im}\left(\frac{\partial\Psi_1^*}{\partial x}\Psi_2 - \Psi_1^*\frac{\partial\Psi_2}{\partial x}\right)\Bigg|_{-\infty}^{\infty}$$

推导到这步给 5 分

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = 0$$

给出正确答案 10 分

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