课堂练习

练习1：证明无限深方势阱中，波函数满足正交关系$\int_0^a \psi_m^*(x)\psi_n(x)dx=\delta_{mn}$，其中$\psi_n(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x)$

证明：当$m=n$时，有：

$$\int_0^a \psi_m^*(x)\psi_n(x)dx=\int_0^a \frac{2}{a}\sin^2(\frac{n\pi}{a}x)dx=\int_0^a \frac{2}{a}\frac{1-\cos(\frac{2n\pi}{a}x)}{2}dx=[\frac{x}{a}-\frac{\sin(\frac{2n\pi}{a}x)}{2n\pi}]_0^a=1$$

当$m\neq n$时，有：

$$\int_0^a \psi_m^*(x)\psi_n(x)dx=\int_0^a \frac{2}{a}\sin(\frac{m\pi}{a}x)\sin(\frac{n\pi}{a}x)dx=\int_0^a \frac{2}{a}\frac{\cos[\frac{(m-n)\pi}{a}x]-\cos[\frac{(m+n)\pi}{a}x]}{2}dx=[\frac{\sin[\frac{(m-n)\pi}{a}x]}{(m-n)\pi}-\frac{\sin[\frac{(m+n)\pi}{a}x]}{(m+n)\pi}]_0^a=0$$

综上可知$\int_0^a \psi_m^*(x)\psi_n(x)dx=\delta_{mn}$

练习2：将箱中粒子的势函数定义为$V(x)=\begin{cases}0 & (|x|<\frac{a}{2})\\ +\infty & (|x|\geq\frac{a}{2})\end{cases}$，写出相应的本征能量和本征波函数

解：由于势能函数$V(x)$为偶函数，因此波函数必满足一定的宇称（即波函数要么为奇函数，要么为偶函数）。又当$|x|<\frac{a}{2}$时，将势能函数代入定态薛定谔方程，得$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$，或$\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi$。记$k=\sqrt{\frac{2mE}{\hbar^2}}$，则波函数的解为$\psi(x)=A\mathrm{e}^{\mathrm{i}kx}+B\mathrm{e}^{-\mathrm{i}kx}\ (|x|<\frac{a}{2})$；当$|x|\geq\frac{a}{2}$时，因$V(x)=+\infty$，故波函数为$\psi(x)=0\ (|x|\geq\frac{a}{2})$。结合波函数的连续性，得$\begin{cases}\psi(\frac{a}{2})=A\mathrm{e}^{\frac{\mathrm{i}ka}{2}}+B\mathrm{e}^{-\frac{\mathrm{i}ka}{2}}=0\\ \psi(-\frac{a}{2})=A\mathrm{e}^{-\frac{\mathrm{i}ka}{2}}+B\mathrm{e}^{\frac{\mathrm{i}ka}{2}}=0\end{cases}$。
接下来，我们联立这两个等式，得$\mathrm{e}^{\mathrm{i}ka}=\mathrm{e}^{-\mathrm{i}ka}$，即$\mathrm{e}^{2\mathrm{i}ka}=1$，从而有$2ka=2n\pi\ (n\in\mathbb{Z}^+)$，即$k=\frac{n\pi}{a}\ (n\in\mathbb{Z}^+)$，相应的，本征能量为$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}$。
将k与n的关系式代回边界条件，得$\begin{cases}\psi(\frac{a}{2})=A\mathrm{e}^{\frac{\mathrm{i}n\pi}{2}}+B\mathrm{e}^{-\frac{\mathrm{i}n\pi}{2}}=0\\ \psi(-\frac{a}{2})=A\mathrm{e}^{-\frac{\mathrm{i}n\pi}{2}}+B\mathrm{e}^{\frac{\mathrm{i}n\pi}{2}}=0\end{cases}$。当$n=2p\ (p\in\mathbb{Z}^+)$时，可得$A+B=0$，即$A=-B$，此时

$$\psi(x)=A(\mathrm{e}^{\mathrm{i}kx}-\mathrm{e}^{-\mathrm{i}kx})=2\mathrm{i}A\sin(kx)=A^{'}\sin(kx)=A^{'}\sin(\frac{n\pi x}{a})=A^{'}\sin(\frac{2p\pi x}{a})\ (|x|<\frac{a}{2})$$

接下来归一化得

$$\int_{-\frac{a}{2}}^{\frac{a}{2}}|\psi(x)|^2dx=\int_{-\frac{a}{2}}^{\frac{a}{2}}|A^{'}|^2\sin^2(kx)dx=[\frac{|A^{'}|^2x}{2}-\frac{|A^{'}|^2\sin(2kx)}{4k}]_{-\frac{a}{2}}^{\frac{a}{2}}=\frac{|A^{'}|^2a}{2}=1$$

即$|A^{'}|=\sqrt{\frac{2}{a}}$，故当$A^{'}$取正实数时，有$\psi_n(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\ (|x|<\frac{a}{2}, n\text{ is even})$，或写作$\psi_p(x)=\sqrt{\frac{2}{a}}\sin(\frac{2p\pi x}{a})\ (|x|<\frac{a}{2}, p\in\mathbb{Z}^+)$，此时本征能量可改写为$E_p=\frac{2p^2\pi^2\hbar^2}{ma^2}\ (p\in\mathbb{Z}^+)$。
当$n=2p-1\ (p\in\mathbb{Z}^+)$时，可得$A-B=0$，即$A=B$，此时

$$\psi(x)=B(\mathrm{e}^{\mathrm{i}kx}+\mathrm{e}^{-\mathrm{i}kx})=2B\cos(kx)=B^{'}\cos(kx)=B^{'}\cos(\frac{n\pi x}{a})=B^{'}\cos[\frac{(2p-1)\pi x}{a}]\ (|x|<\frac{a}{2})$$

接下来归一化得

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} |\psi(x)|^2 dx = \int_{-\frac{a}{2}}^{\frac{a}{2}} |B^{'}|^2 \cos^2(kx)dx = [\frac{|B^{'}|^2 x}{2} + \frac{|B^{'}|^2 \sin(2kx)}{4k}]_{-\frac{a}{2}}^{\frac{a}{2}} = \frac{|B^{'}|^2 a}{2} = 1$$

即$|B^{'}| = \sqrt{\frac{2}{a}}$，故当$B^{'}$取正实数时，有$\psi_n(x) = \sqrt{\frac{2}{a}}\cos(\frac{n\pi x}{a})$ $(|x| < \frac{a}{2}, n \text{ is odd})$，或写作$\psi_p(x) = \sqrt{\frac{2}{a}}\cos[\frac{(2p-1)\pi x}{a}]$ $(|x| < \frac{a}{2}, p \in \mathbb{Z}^+)$，此时本征能量可改写为$E_p = \frac{(2p-1)^2\pi^2\hbar^2}{2ma^2}$ $(p \in \mathbb{Z}^+)$。

综上，本征波函数为$\psi(x) = \sqrt{\frac{2}{a}} \cdot \begin{cases} \cos(\frac{n\pi x}{a}) \text{ when } n \text{ is odd} \\ \sin(\frac{n\pi x}{a}) \text{ when } n \text{ is even} \end{cases}$ $(|x| < \frac{a}{2}, n \in \mathbb{Z}^+)$，相应的本征能量为$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ $(n \in \mathbb{Z}^+)$。

练习3：求湮灭（湮没）算符$\hat{a}$和创造（产生）算符$\hat{a}^\dagger$的对易关系$[\hat{a}, \hat{a}^\dagger]$

解：我们知道$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega})$，$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega})$，因此：

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega}) \cdot \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega}) - \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega}) \cdot \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega}) \\
&= \frac{m\omega}{2\hbar}[(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega})(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega}) - (\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega})(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega})] = \frac{m\omega}{2\hbar}[(\hat{x}^2 + \frac{\mathrm{i}\hat{p}\hat{x}}{m\omega} - \frac{\mathrm{i}\hat{x}\hat{p}}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2}) - (\hat{x}^2 - \frac{\mathrm{i}\hat{p}\hat{x}}{m\omega} + \frac{\mathrm{i}\hat{x}\hat{p}}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2})] \\
&= \frac{m\omega}{2\hbar}(-\frac{2\mathrm{i}}{m\omega})(\hat{x}\hat{p} - \hat{p}\hat{x}) = \frac{m\omega}{2\hbar}(-\frac{2\mathrm{i}}{m\omega})\mathrm{i}\hbar = 1
\end{aligned}$$

练习4：证明如下等式：$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

证明：我们知道占据数算符定义为$\hat{N} = \hat{a}^\dagger\hat{a}$，它满足$\hat{N}|n\rangle = n|n\rangle$。又根据湮没算符和产生算符满足$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$，因此$\hat{N}^\dagger = \hat{a}\hat{a}^\dagger = \hat{N} + 1$。另一方面，由于

$$\begin{aligned}
\hat{N}\hat{a}^\dagger|n\rangle &= ([\hat{N}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{N})|n\rangle = [\hat{N}, \hat{a}^\dagger]|n\rangle + \hat{a}^\dagger\hat{N}|n\rangle = [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger]|n\rangle + \hat{a}^\dagger\hat{N}|n\rangle = (\hat{a}^\dagger[\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}^\dagger]\hat{a})|n\rangle + \hat{a}^\dagger\hat{N}|n\rangle \\
&= (\hat{a}^\dagger \cdot 1 + 0 \cdot \hat{a})|n\rangle + \hat{a}^\dagger\hat{N}|n\rangle = \hat{a}^\dagger|n\rangle + n\hat{a}^\dagger|n\rangle = (n+1)\hat{a}|n\rangle
\end{aligned}$$

故$\begin{cases} \hat{a}^\dagger|n\rangle = c_\uparrow|n+1\rangle \\ \langle n|\hat{a} = \langle n+1|c_\uparrow^* \end{cases}$，从而$(\langle n|\hat{a})(\hat{a}^\dagger|n\rangle) = (\langle n+1|c_\uparrow^*)(c_\uparrow|n+1\rangle) = |c_\uparrow|^2$，结合$(\langle n|\hat{a})(\hat{a}^\dagger|n\rangle) = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|(\hat{N}+1)|n\rangle = n+1$，得$|c_\uparrow|^2 = n+1$，即$|c_\uparrow| = \sqrt{n+1}$，当$c_\uparrow$为正实数时，即有$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$，证毕