课堂练习

练习1：考虑电子自旋在均匀磁场中的进动，设电子在$t=0$的状态为$|u(0)\rangle=|S_x+\rangle=\frac{1}{\sqrt{2}}(|S_z+\rangle+|S_z-\rangle)$，试证明$t$时刻各个自旋算符的期望值为$\langle S_x\rangle(t)=\frac{\hbar}{2}\cos\omega t$，$\langle S_y\rangle(t)=\frac{\hbar}{2}\sin\omega t$，$\langle S_z\rangle(t)=0$

证明：由于

$$|u(t)\rangle=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|u(0)\rangle=\mathrm{e}^{-\frac{\mathrm{i}\omega t}{\hbar}\hat{S}_z}\Big[\frac{1}{\sqrt{2}}(|S_z+\rangle+|S_z-\rangle)\Big]=\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)$$

故代入得：

$$\begin{aligned}\langle S_x\rangle(t)&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\hat{S}_x\Big[\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\Big]\\&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\frac{1}{2}(\hat{S}_++\hat{S}_-)\Big[\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\Big]\\&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\frac{\hbar}{2\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\\&=\frac{\hbar}{4}(\mathrm{e}^{\mathrm{i}\omega t}\langle S_z+|S_z+\rangle+\langle S_z-|S_z+\rangle+\langle S_z+|S_z-\rangle+\mathrm{e}^{-\mathrm{i}\omega t}\langle S_z-|S_z-\rangle)\\&=\frac{\hbar}{4}(\cos\omega t+\mathrm{i}\sin\omega t+\cos\omega t-\mathrm{i}\sin\omega t)=\frac{\hbar}{2}\cos\omega t\end{aligned}$$

$$\begin{aligned}\langle S_y\rangle(t)&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\hat{S}_y\Big[\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\Big]\\&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\frac{1}{2\mathrm{i}}(\hat{S}_+-\hat{S}_-)\Big[\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\Big]\\&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\frac{\hbar}{2\sqrt{2}\mathrm{i}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle-\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\\&=\frac{\hbar}{4\mathrm{i}}(\mathrm{e}^{\mathrm{i}\omega t}\langle S_z+|S_z+\rangle+\langle S_z-|S_z+\rangle-\langle S_z+|S_z-\rangle-\mathrm{e}^{-\mathrm{i}\omega t}\langle S_z-|S_z-\rangle)\\&=\frac{\hbar}{4\mathrm{i}}(\cos\omega t+\mathrm{i}\sin\omega t-\cos\omega t+\mathrm{i}\sin\omega t)=\frac{\hbar}{2}\sin\omega t\end{aligned}$$

$$\begin{aligned}\langle S_z\rangle(t)&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{\frac{-\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\hat{S}_z\Big[\frac{1}{\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle+\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\Big]\\&=\frac{1}{\sqrt{2}}(\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}\langle S_z+|+\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}\langle S_z-|)\cdot\frac{\hbar}{2\sqrt{2}}(\mathrm{e}^{-\frac{\mathrm{i}\omega t}{2}}|S_z+\rangle-\mathrm{e}^{\frac{\mathrm{i}\omega t}{2}}|S_z-\rangle)\\&=\frac{\hbar}{4}(\langle S_z+|S_z+\rangle+\mathrm{e}^{-\mathrm{i}\omega t}\langle S_z-|S_z+\rangle-\mathrm{e}^{\mathrm{i}\omega t}\langle S_z+|S_z-\rangle-\langle S_z-|S_z-\rangle)=0\end{aligned}$$

练习2：验证任意时刻态矢$|u(t)\rangle$在$\hat{B}$的本征态$\{|b_i\rangle\}$上的展开系数在两种表象中是一样的

解：在薛定谔表象下，态矢$|u(t)\rangle_S=\hat{U}(t)|u(0)\rangle$，将该态矢展开，得$|u(t)\rangle_S=\sum\limits_i|b_i\rangle\langle b_i|\hat{U}(t)|u(0)\rangle$，因此展开系数为$c_i^{(S)}=\langle b_i|\hat{U}(t)|u(0)\rangle$；
另一方面，薛定谔表象下的本征方程为$\hat{B}|b_i(0)\rangle_S=b_i|b_i(0)\rangle_S$，记$|b_i(0)\rangle_S=|b_i\rangle$，则本征方程可改写为$\hat{B}|b_i\rangle=b_i|b_i\rangle$，左乘$\hat{U}^\dagger(t)$，得$\hat{U}^\dagger(t)\hat{B}|b_i\rangle=\hat{U}^\dagger(t)\hat{B}\hat{U}(t)\hat{U}^\dagger(t)|b_i\rangle=b_i\hat{U}^\dagger(t)|b_i\rangle$，再记$\hat{B}_H(t)=\hat{U}^\dagger(t)\hat{B}\hat{U}(t)$，$|b_i(t)\rangle_H=\hat{U}^\dagger(t)|b_i(t)\rangle$，则海森堡表象下的本征方程为$\hat{B}_H(t)|b_i(t)\rangle=b_i|b_i(t)\rangle$；
回到本题，在海森堡表象下，态矢$|u(t)\rangle_H=|u(0)\rangle$，不随时间而改变，将该态矢展开，得

$|u(t)\rangle_H=\sum_i|b_i(t)\rangle_H\langle b_i(t)|_H\cdot|u(0)\rangle=\sum_i|b_i(t)\rangle_H\langle b_i|\hat{U}|u(0)\rangle$，因此展开系数为 $c_i^{(H)}=\langle b_i|\hat{U}(t)|u(0)\rangle=c_i^{(S)}$，原题得证

练习3：已知从银炉中出来的银原子，有$\frac{1}{2}$的概率为自旋向上（即$|S_z+\rangle$），有$\frac{1}{2}$的概率为自旋向上（即$|S_z-\rangle$），试验证其密度算符可写作 $\hat{\rho}=\frac{1}{2}(|S_x+\rangle\langle S_x+|+|S_x-\rangle\langle S_x-|)$

解：根据题意，密度算符为$\hat{\rho}=\frac{1}{2}(|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z-|)$；另一方面，由于 $|S_x\pm\rangle=\frac{1}{\sqrt{2}}(|S_z+\rangle\pm|S_z-\rangle)$，故：

$$\begin{aligned}|S_x+\rangle\langle S_x+|&=\frac{1}{\sqrt{2}}(|S_z+\rangle+|S_z-\rangle)\cdot\frac{1}{\sqrt{2}}(\langle S_z+|+\langle S_z-|)\\&=\frac{1}{2}(|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z+|+|S_z+\rangle\langle S_z-|+|S_z-\rangle\langle S_z-|)\end{aligned}$$

$$\begin{aligned}|S_x-\rangle\langle S_x-|&=\frac{1}{\sqrt{2}}(|S_z+\rangle-|S_z-\rangle)\cdot\frac{1}{\sqrt{2}}(\langle S_z+|-\langle S_z-|)\\&=\frac{1}{2}(|S_z+\rangle\langle S_z+|-|S_z-\rangle\langle S_z+|-|S_z+\rangle\langle S_z-|+|S_z-\rangle\langle S_z-|)\end{aligned}$$

从而有

$$\begin{aligned}|S_x+\rangle\langle S_x+|+|S_x-\rangle\langle S_x-|=&\frac{1}{2}(|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z+|+|S_z+\rangle\langle S_z-|+|S_z-\rangle\langle S_z-|)\\&+\frac{1}{2}(|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z+|+|S_z+\rangle\langle S_z-|+|S_z-\rangle\langle S_z-|)\\=&|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z-|\end{aligned}$$

故代回密度算符的表达式，得$\hat{\rho}=\frac{1}{2}(|S_x+\rangle\langle S_x+|+|S_x-\rangle\langle S_x-|)$

练习4：纯态$|S_x+\rangle$所对应的密度算符是什么？

解：（用方程表示）因为$|S_x+\rangle=\frac{1}{\sqrt{2}}(|S_z+\rangle+|S_z-\rangle)$，所以相应的密度算符为

$$\begin{aligned}\hat{\rho}=|S_x+\rangle\langle S_x+|&=\frac{1}{\sqrt{2}}(|S_z+\rangle+|S_z-\rangle)\cdot\frac{1}{\sqrt{2}}(\langle S_z+|+\langle S_z-|)\\&=\frac{1}{2}(|S_z+\rangle\langle S_z+|+|S_z-\rangle\langle S_z+|+|S_z+\rangle\langle S_z-|+|S_z-\rangle\langle S_z-|)\end{aligned}$$

（用矩阵表示）因为$|S_x+\rangle$可表示为$|S_x+\rangle=\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$，所以密度算符可表示为

$$\hat{\rho}=|S_x+\rangle\langle S_x+|=\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{2}}\end{bmatrix}=\frac{1}{2}\begin{bmatrix}1&1\\1&1\end{bmatrix}$$

练习5：证明对于任意状态（无论是纯态还是混合态），总有$\mathrm{Tr}(\hat{\rho}^2)\leq 1$

证明：在任意基组$\{|u_i\rangle\}$下，有

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}^2)&=\sum_i\langle u_i|\hat{\rho}^2|u_i\rangle=\sum_i\langle u_i|(\sum_j\omega_j|\beta_j\rangle\langle\beta_j|\sum_k\omega_k|\beta_k\rangle\langle\beta_k|)|u_i\rangle=\sum_{i,j,k}\omega_j\omega_k\langle u_i|\beta_j\rangle\langle\beta_j|\beta_k\rangle\langle\beta_k|u_i\rangle\\&=\sum_{j,k}\omega_j\omega_k\langle\beta_j|\beta_k\rangle(\sum_i\langle\beta_k|u_i\rangle\langle u_i|\beta_j\rangle)=\sum_{j,k}\omega_j\omega_k\langle\beta_j|\beta_k\rangle\langle\beta_k|\beta_j\rangle\leq\sum_{j,k}\omega_j\omega_k\langle\beta_j|\beta_j\rangle\langle\beta_k|\beta_k\rangle\\&=(\sum_j\omega_j\langle\beta_j|\beta_j\rangle)(\sum_k\omega_k\langle\beta_k|\beta_k\rangle)=\sum_j\omega_j\sum_k\omega_k=1\end{aligned}$$

等式成立的条件为该密度算符中出现的所有$|\beta_i\rangle$之间仅相差一个相因子，也即该密度算符表征一个纯态。对混合态，上式小于号成立。