

第十一周作业答案

1. 我们用 $|\varphi_n\rangle$ 表示厄米算符 H 的本征态（譬如， H 可以是任何物理体系的哈密顿算符），假设全体 $|\varphi_n\rangle$ 构成一个离散的正交归一基。算符 $U(m, n)$ 定义是

$$U(m, n) = |\varphi_m\rangle\langle\varphi_n|,$$

- 计算 $U(m, n)$ 的伴随算符 $U^\dagger(m, n)$,
- 计算对易子 $[H, U(m, n)]$,
- 证明:

$$U(m, n)U^\dagger(p, q) = \delta_{n,q}U(m, p),$$

- 计算算符 $U(m, n)$ 的迹 $\text{Tr}\{U(m, n)\}$,
- 设 A 是一个算符，它的矩阵元是 $A_{mn} = \langle\varphi_m|A|\varphi_n\rangle$ ；试证：

$$A = \sum_{m,n} A_{mn}U(m, n),$$

- 试证： $A_{pq} = \text{Tr}\{AU^\dagger(p, q)\}$ 。

解：

a.

$$U^\dagger(m, n) = (|\varphi_m\rangle\langle\varphi_n|)^\dagger = |\varphi_n\rangle\langle\varphi_m|.$$

b.

因为 $H|\varphi_n\rangle = \lambda_n|\varphi_n\rangle$,

所以 $\langle\varphi_n|H^\dagger = \lambda_n^*\langle\varphi_n|$ ，也就是 $\langle\varphi_n|H = \lambda_n^*\langle\varphi_n|$

$$\begin{aligned} [H, U(m, n)] &= H|\varphi_m\rangle\langle\varphi_n| - |\varphi_m\rangle\langle\varphi_n|H \\ &= \lambda_m|\varphi_m\rangle\langle\varphi_n| - \lambda_n^*|\varphi_m\rangle\langle\varphi_n| \\ &= (\lambda_m - \lambda_n)U(m, n), \end{aligned}$$

其中 $\lambda_{m,n}$ 是 $|\varphi_{m,n}\rangle$ 态对应的本征值，且厄米算符的本征值为实数。

c.

$$\begin{aligned} U(m, n)U^\dagger(p, q) &= |\varphi_m\rangle\langle\varphi_n|(|\varphi_p\rangle\langle\varphi_q|)^\dagger \\ &= |\varphi_m\rangle\langle\varphi_n|\varphi_q\rangle\langle\varphi_p| \\ &= \delta_{n,q}|\varphi_m\rangle\langle\varphi_p| = \delta_{n,q}U(m, p). \end{aligned}$$

d.

$$\text{Tr}\{U(m, n)\} = \sum_n \langle\varphi_n|U(m, n)|\varphi_n\rangle = \sum_n 1 = N.$$

N 是 $\{|\varphi_n\rangle\}$ 这一离散正交归一基的维度（总数）

- 利用态空间中恒等算符的表达式

$$A = \sum_m |\varphi_m\rangle\langle\varphi_m|A\sum_n |\varphi_n\rangle\langle\varphi_n|$$

$$\begin{aligned}
&= \sum_{m,n} |\varphi_m\rangle \langle \varphi_m| A |\varphi_n\rangle \langle \varphi_n| \\
&= \sum_{m,n} A_{mn} |\varphi_m\rangle \langle \varphi_n| \\
&= \sum_{m,n} A_{mn} U(m, n).
\end{aligned}$$

f.

$$\begin{aligned}
\text{Tr}\{AU^\dagger(p, q)\} &= \sum_n \langle \varphi_n | AU^\dagger(p, q) | \varphi_n \rangle \\
&= \sum_n \langle \varphi_n | A | \varphi_q \rangle \langle \varphi_p | \varphi_n \rangle \\
&= \sum_n \langle \varphi_n | A | \varphi_q \rangle \delta_{np} = A_{pq}.
\end{aligned}$$

2. 在一个二维矢量空间中，考虑这样一个算符，它在正交归一基 $\{|1\rangle, |2\rangle\}$ 中的矩阵为：

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

- σ_y 是厄米算符吗？试计算它的本征值和本征矢（要给出它们在基 $\{|1\rangle, |2\rangle\}$ 中的已归一化的展开式）。
- 计算在这些本征矢上的投影算符的矩阵，然后证明它们满足正交归一关系式和封闭性关系式。
- 同样是上面这些问题，但矩阵为三维空间的矩阵

$$L_y = \frac{\hbar}{2i} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}.$$

解：

a.

$$\sigma_y^\dagger = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y,$$

即 σ_y 是厄米算符。

用特征方程求解算符的本征值和本征矢：

$$\sigma_y |\psi\rangle = \lambda |\psi\rangle,$$

$$\sum_m \langle n | \sigma_y | m \rangle \langle m | \psi \rangle = \lambda \langle n | \psi \rangle,$$

$$\sum_m \langle n | \sigma_y | m \rangle c_m = \lambda c_n, \quad c_n = \langle n | \psi \rangle,$$

$$\text{Det}(\sigma_y - \lambda I) = \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = 0,$$

$$\lambda^2 - 1 = 0, \quad \lambda_{\pm} = \pm 1,$$

$$i c_{1\pm} - \lambda_{\pm} c_{2\pm} = 0,$$

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + i|2\rangle),$$

$$|\psi_-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - i|2\rangle).$$

b. 投影算符 $P_{\psi_{\pm}} = |\psi_{\pm}\rangle\langle\psi_{\pm}|$ 的矩阵元为

$$\langle m | P_{\psi_{\pm}} | n \rangle = \langle m | \psi_{\pm} \rangle \langle \psi_{\pm} | n \rangle = c_{m\pm} c_{n\pm}^*,$$

矩阵表示为

$$P_{\psi_+} = |\psi_+\rangle\langle\psi_+| = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ i & \frac{1}{2} \end{pmatrix},$$

$$P_{\psi_-} = |\psi_-\rangle\langle\psi_-| = \begin{pmatrix} \frac{1}{2} & i \\ -\frac{i}{2} & \frac{1}{2} \end{pmatrix}.$$

$\{|\psi_+\rangle, |\psi_-\rangle\}$ 正交归一性:

$$\langle \psi_{\alpha} | \psi_{\alpha} \rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\alpha \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \alpha \frac{i}{\sqrt{2}} \end{pmatrix} = 1, \quad \alpha = \pm,$$

$$\langle \psi_+ | \psi_- \rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix} = \langle \psi_- | \psi_+ \rangle^* = 0,$$

$$\langle \psi_{\alpha} | \psi_{\beta} \rangle = \delta_{\alpha\beta}.$$

封闭性关系

$$P_{\{|\psi_+\rangle, |\psi_-\rangle\}} = \sum_{\alpha} |\psi_{\alpha}\rangle\langle\psi_{\alpha}| = P_{\psi_+} + P_{\psi_-}$$

$$\begin{aligned}
&= \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ i & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I.
\end{aligned}$$

即 $\{|\psi_+\rangle, |\psi_-\rangle\}$ 满足正交归一关系式和封闭性关系式。

c. 对于 $L_y = \frac{\hbar}{2i} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}$,

$$L_y^\dagger = -\frac{\hbar}{2i} \begin{pmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} = L_y,$$

求解本征值

$$\text{Det}(L_y - \lambda I) = \frac{\hbar}{2i} \begin{vmatrix} -2i\lambda/\hbar & \sqrt{2} & 0 \\ -\sqrt{2} & -2i\lambda/\hbar & \sqrt{2} \\ 0 & -\sqrt{2} & -2i\lambda/\hbar \end{vmatrix} = 0,$$

$$-\frac{2i\lambda}{\hbar} \left(-\frac{4\lambda^2}{\hbar^2} + 2 \right) - \frac{4i\lambda}{\hbar} = \frac{2i\lambda}{\hbar} \left(\frac{4\lambda^2}{\hbar^2} - 4 \right) = 0,$$

$$\lambda_1 = \hbar, \quad |\psi_1\rangle = \frac{1}{2} (|1\rangle + i\sqrt{2}|2\rangle - |3\rangle),$$

$$\lambda_2 = 0, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |3\rangle),$$

$$\lambda_3 = -\hbar, \quad |\psi_3\rangle = \frac{1}{2} (|1\rangle - i\sqrt{2}|2\rangle - |3\rangle),$$

投影算符为

$$P_{\psi_1} = |\psi_1\rangle\langle\psi_1| = \begin{pmatrix} \frac{1}{4} & -i\frac{\sqrt{2}}{4} & -\frac{1}{4} \\ i\frac{\sqrt{2}}{4} & \frac{1}{2} & -i\frac{\sqrt{2}}{4} \\ -\frac{1}{4} & i\frac{\sqrt{2}}{4} & \frac{1}{4} \end{pmatrix},$$

$$P_{\psi_2} = |\psi_2\rangle\langle\psi_2| = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix},$$

$$P_{\psi_3} = |\psi_3\rangle\langle\psi_3| = \begin{pmatrix} \frac{1}{4} & i\frac{\sqrt{2}}{4} & -\frac{1}{4} \\ -i\frac{\sqrt{2}}{4} & \frac{1}{2} & i\frac{\sqrt{2}}{4} \\ -\frac{1}{4} & -i\frac{\sqrt{2}}{4} & \frac{1}{4} \end{pmatrix},$$

证明 $\{|\psi_i\rangle\}$ 满足正交归一关系式和封闭性关系式:

$$\langle\psi_i|\psi_i\rangle = \sum_n \langle\psi_i|n\rangle\langle n|\psi_i\rangle = \sum_n |\langle n|\psi_i\rangle|^2 = 1, \quad i = 1, 2, 3$$

$$\langle\psi_1|\psi_2\rangle = \begin{pmatrix} \frac{1}{2} & -\frac{i}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 1 \end{pmatrix} = \langle\psi_2|\psi_1\rangle^* = 0,$$

$$\langle\psi_3|\psi_2\rangle = \begin{pmatrix} \frac{1}{2} & \frac{i}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 1 \end{pmatrix} = \langle\psi_2|\psi_3\rangle^* = 0,$$

$$\langle\psi_1|\psi_3\rangle = \begin{pmatrix} \frac{1}{2} & -\frac{i}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ -\frac{i}{\sqrt{2}} \\ -\frac{1}{2} \end{pmatrix} = \langle\psi_3|\psi_1\rangle^* = 0,$$

$$\langle\psi_i|\psi_j\rangle = \delta_{ij},$$

$$P_{\{|\psi_i\rangle\}} = \sum_i |\psi_i\rangle\langle\psi_i| = P_{\psi_1} + P_{\psi_2} + P_{\psi_3}$$

$$\begin{aligned} &= \begin{pmatrix} \frac{1}{4} & -i\frac{\sqrt{2}}{4} & -\frac{1}{4} \\ i\frac{\sqrt{2}}{4} & \frac{1}{2} & -i\frac{\sqrt{2}}{4} \\ -\frac{1}{4} & i\frac{\sqrt{2}}{4} & \frac{1}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} & i\frac{\sqrt{2}}{4} & -\frac{1}{4} \\ -i\frac{\sqrt{2}}{4} & \frac{1}{2} & i\frac{\sqrt{2}}{4} \\ -\frac{1}{4} & -i\frac{\sqrt{2}}{4} & \frac{1}{4} \end{pmatrix} \\ &= I. \end{aligned}$$

3. 矩阵 σ_x 的定义为:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

试证：

$$e^{i\alpha\sigma_x} = I \cos \alpha + i\sigma_x \sin \alpha,$$

其中 I 是 2×2 单位矩阵。

证明

$$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I,$$

$$\sigma_x^{2n+1} = \sigma_x,$$

$$\sigma_x^{2n} = I,$$

$$e^{i\alpha\sigma_x} = \sum_n \frac{i^n}{n!} \alpha^n \sigma_x^n$$

$$= \sum_n \frac{i^{2n}}{(2n)!} \alpha^{2n} \sigma_x^{2n} + \sum_n \frac{i^{2n+1}}{(2n+1)!} \alpha^{2n+1} \sigma_x^{2n+1}$$

$$= \sum_n \frac{i^{2n}}{(2n)!} \alpha^{2n} I + \sum_n \frac{i^{2n+1}}{(2n+1)!} \alpha^{2n+1} \sigma_x$$

$$= I \cos \alpha + i\sigma_x \sin \alpha.$$