

## 课堂练习

### 练习1: 证明任意矢量用一组基矢的展开是唯一的

**证明:** 反证法, 设 $|\alpha\rangle$ 在基矢 $\{|u_i\rangle\}$ 下存在至少两种展开 $|\alpha\rangle = \sum_{i=1}^n \alpha_i |u_i\rangle = \sum_{i=1}^n \alpha'_i |u_i\rangle$ , 其中 $\alpha_i$ 与 $\alpha'_i$ 不全相等, 则移项得 $\sum_{i=1}^n (\alpha_i - \alpha'_i) |u_i\rangle = 0$ , 若第 $k_1, k_2, \dots, k_m$ 项满足 $\alpha_{k_1} \neq \alpha'_{k_1}, \alpha_{k_2} \neq \alpha'_{k_2}, \dots, \alpha_{k_m} \neq \alpha'_{k_m}$ , 原式可化为 $\sum_{i=1}^n (\alpha_{k_i} - \alpha'_{k_i}) |u_{k_i}\rangle = 0$ , 即 $|u_{k_1}\rangle, |u_{k_2}\rangle, \dots, |u_{k_m}\rangle$ 线性相关, 但基矢 $\{|u_i\rangle\}$ 之间满足线性无关, 矛盾! 因此任意矢量用一组基矢的展开是唯一的。

### 练习2: 证明 $S_{1/2}$ 是个二维的复数线性空间

**证明:** 易知 $S_2$ 是个二维的复数线性空间 $\Leftrightarrow$ 线性无关的向量(右矢)个数最多有两个, 故先设两个右矢:  $|a\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$ ,  $|b\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$ , 满足 $n_a |a\rangle + n_b |b\rangle = 0$ , 则有 $\begin{cases} n_a a_1 + n_b b_1 = 0 \\ n_a a_2 + n_b b_2 = 0 \end{cases}$ , 由此得 $\begin{cases} n_b(b_1 a_2 - b_2 a_1) = 0 \\ n_b(a_1 b_2 - a_2 b_1) = 0 \end{cases}$ . 对以上情形, 只要保证 $\begin{cases} a_1, a_2, b_1, b_2 \neq 0 \\ a_1 b_2 \neq b_1 a_2 \end{cases}$ , 即可得到 $n_a = n_b = 0$ , 从而 $|a\rangle$ 与 $|b\rangle$ 线性无关, 即 $S_2$ 中线性无关的向量(右矢)个数可以为两个。

接下来, 我们还要证明 $S_2$ 中线性无关的向量(右矢)个数不能为三个或更多个。设三个右矢:

$|a\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$ ,  $|b\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$ ,  $|c\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$ , 满足 $n_a |a\rangle + n_b |b\rangle + n_c |c\rangle = 0$ , 则有 $\begin{cases} n_a a_1 + n_b b_1 + n_c c_1 = 0 \\ n_a a_2 + n_b b_2 + n_c c_2 = 0 \end{cases}$ , 该方程组中齐次线性方程的个数小于变量个数, 故有无穷组非零解, 从而存在不全为零的 $n_a, n_b, n_c$ , 使 $n_a |a\rangle + n_b |b\rangle + n_c |c\rangle = 0$ , 即 $|a\rangle, |b\rangle, |c\rangle$ 线性相关。对更多右矢的情形, 同理可证它们均满足线性相关。

综上,  $S_2$ 是个二维的复数线性空间。

注: 如果不用线性方程组的性质, 第二部分亦可按如下说明: 由 $\begin{cases} n_a a_1 + n_b b_1 + n_c c_1 = 0 \\ n_a a_2 + n_b b_2 + n_c c_2 = 0 \end{cases}$ , 得 $\begin{cases} n_b(b_1 a_2 - b_2 a_1) + n_c(c_1 a_2 - c_2 a_1) = 0 \\ n_a(a_1 b_2 - a_2 b_1) + n_c(c_1 b_2 - c_2 b_1) = 0 \\ n_a(a_1 c_2 - a_2 c_1) + n_b(b_1 c_2 - b_2 c_1) = 0 \end{cases}$ , 若 $|a\rangle, |b\rangle, |c\rangle$ 线性无关, 则前提条件为 $\begin{cases} a_1 b_2 \neq a_2 b_1 \\ b_1 c_2 \neq b_2 c_1 \\ c_1 a_2 \neq c_2 a_1 \end{cases}$  (否则在 $|a\rangle, |b\rangle, |c\rangle$ 中取任意一对向量, 必满足线性相关, 矛盾!), 此时可得到如下比例关系: $n_a : n_b : n_c = (b_1 c_2 - b_2 c_1) : (c_1 a_2 - c_2 a_1) : (a_1 b_2 - a_2 b_1)$ , 从而存在不全为零的 $n_a, n_b, n_c$ , 使 $n_a |a\rangle + n_b |b\rangle + n_c |c\rangle = 0$ , 即 $|a\rangle, |b\rangle, |c\rangle$ 线性相关, 这与 $|a\rangle, |b\rangle, |c\rangle$ 线性无关矛盾。对更多右矢的情形, 同理可证它们均满足线性相关。

### 练习3: 证明基矢 $\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a}x)$ , $n = 1, 2, 3, \dots$ 是正交归一的

**证明:** 证明过程可分为两部分:

#### 1. 正交

取两个不相同的基矢 $\psi_m(x)$ 和 $\psi_n(x)$ , 其中 $m \neq n$ , 则其内积为:

$$\begin{aligned} \langle \psi_m | \psi_n \rangle &= \int_0^a \psi_m^*(x) \psi_n(x) dx = \int_0^a \frac{2}{a} \sin\left(\frac{m\pi}{a}x\right) \sin\left(\frac{n\pi}{a}x\right) dx = \int_0^a \frac{1}{a} \left[ \cos \frac{(m-n)\pi}{a}x - \cos \frac{(m+n)\pi}{a}x \right] dx \\ &= \left[ \frac{1}{(m-n)\pi} \sin \frac{(m-n)\pi}{a}x - \frac{1}{(m+n)\pi} \sin \frac{(m+n)\pi}{a}x \right]_0^a = 0 - 0 = 0 \end{aligned}$$

## 2. 归一

对基矢 $\psi_n(x)$ , 求其与自身的内积, 得:

$$\begin{aligned}\langle \psi_n | \psi_n \rangle &= \int_0^a \psi_n^*(x) \psi_n(x) dx = \int_0^a \frac{2}{a} \sin^2\left(\frac{n\pi}{a}x\right) dx = \int_0^a \frac{1}{a} (1 - \cos \frac{2n\pi}{a}x) dx \\ &= \left[ \frac{x}{a} - \frac{1}{2n\pi} \sin \frac{2n\pi}{a}x \right]_0^a = 1 - 0 = 1\end{aligned}$$

综上, 原命题得证。

## 练习4: 推导出Gram-Schmidt正交归一化过程中 $\alpha_2$ 的表达式

解: 易知 $|\phi_2\rangle = \alpha_2(|u_2\rangle - |\phi_1\rangle\langle\phi_1|u_2\rangle)$ , 该基矢满足正交归一条件, 即 $\langle\phi_2|\phi_2\rangle = 1$ , 从而代入得:

$$\begin{aligned}\alpha_2^*(\langle u_2| - \langle u_2|\phi_1\rangle\langle\phi_1|) \cdot \alpha_2(|u_2\rangle - |\phi_1\rangle\langle\phi_1|u_2\rangle) &= |\alpha_2|^2(\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle + \langle u_2|\phi_1\rangle\langle\phi_1|\phi_1\rangle\langle\phi_1|u_2\rangle) \\ &= |\alpha_2|^2(\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle) = 1 \quad (\text{利用 } \langle\phi_1|\phi_1\rangle = 1)\end{aligned}$$

因此 $|\alpha_2|^2 = \frac{1}{\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle}$ , 即 $\alpha_2$ 的模为 $|\alpha_2| = (\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle)^{-1/2}$ , 当然, 由于我们无法得知 $\alpha_2$ 的相位角, 故无法写出 $\alpha_2$ 的具体形式

## 练习5: 证明Gram-Schmidt正交归一化过程中 $\alpha_k$ 的表达式为

$$\alpha_k = [\langle u_k | u_k \rangle - \sum_{i=1}^{k-1} \langle u_k | \varphi_i \rangle \langle \varphi_i | u_k \rangle]^{-\frac{1}{2}}$$

证明: 该式最好与 $|\varphi_k\rangle = \alpha_k(|u_k\rangle - \sum_{i=1}^{k-1} |\varphi_i\rangle\langle\varphi_i|u_k\rangle)$ 一起证明, 此处 $|\varphi_k\rangle$ 已归一化。首先, 我们可以

得知 $|\varphi_1\rangle = |u_1\rangle \cdot \langle u_1|u_1\rangle^{-\frac{1}{2}} = \alpha_1|u_1\rangle$ , 并且 $|\varphi_2\rangle = \alpha_2(|u_2\rangle - |\varphi_1\rangle\langle\varphi_1|u_2\rangle)$ , 其中 $|\alpha_2| = (\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle)^{-1/2}$ , 当 $\alpha_2$ 取实数时, 有 $\alpha_2 = (\langle u_2|u_2\rangle - \langle u_2|\phi_1\rangle\langle\phi_1|u_2\rangle)^{-1/2}$ 。然后, 我们假设 $|\varphi_k\rangle$ 和 $\alpha_k$ 的表达式在 $k=l$ 时成立, 则对 $|u_{l+1}\rangle$ 正交归一化时, 设

$|\varphi_{l+1}\rangle = \alpha_{l+1}|u_{l+1}\rangle + \sum_{i=1}^l \beta_i|\varphi_i\rangle$ , 结合 $\langle\varphi_j|\varphi_{l+1}\rangle = 0 \ (j=1, 2, \dots, l)$ 得:

$$\langle\varphi_j|\varphi_{l+1}\rangle = \langle\varphi_j| \cdot (\alpha_{l+1}|u_{l+1}\rangle + \sum_{i=1}^l \beta_i|\varphi_i\rangle) = \alpha_{l+1}\langle\varphi_j|u_{l+1}\rangle + \sum_{i=1}^l \beta_i\delta_{ji} = 0$$

因此 $\beta_j = -\alpha_{l+1}\langle\varphi_j|u_{l+1}\rangle$ , 代回 $|\varphi_{l+1}\rangle = \alpha_{l+1}|u_{l+1}\rangle + \beta|\varphi_l\rangle$ 得

$|\varphi_{l+1}\rangle = \alpha_{l+1}(|u_{l+1}\rangle - \sum_{i=1}^l |\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle)$ , 又由归一化条件知 $\langle\varphi_{l+1}|\varphi_{l+1}\rangle = 1$ , 因此有:

$$\begin{aligned}\langle\varphi_{l+1}|\varphi_{l+1}\rangle &= \alpha_{l+1}^*(\langle u_{l+1}| - \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|) \cdot \alpha_{l+1}(|u_{l+1}\rangle - \sum_{i=1}^l |\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle) \\ &= |\alpha_{l+1}|^2(\langle u_{l+1}|u_{l+1}\rangle - 2 \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle + \sum_{i=1}^l \sum_{j=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|\varphi_j\rangle\langle\varphi_j|u_{l+1}\rangle) \\ &= |\alpha_{l+1}|^2(\langle u_{l+1}|u_{l+1}\rangle - 2 \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle + \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle) \quad (\text{根据克罗内克符号的性质}) \\ &= |\alpha_{l+1}|^2(\langle u_{l+1}|u_{l+1}\rangle - \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle) = 1\end{aligned}$$

从而 $|\alpha_{l+1}| = [\langle u_{l+1}|u_{l+1}\rangle - \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle]^{-\frac{1}{2}}$ , 当 $\alpha_{l+1}$ 取实数时, 有

$\alpha_{l+1} = [\langle u_{l+1}|u_{l+1}\rangle - \sum_{i=1}^l \langle u_{l+1}|\varphi_i\rangle\langle\varphi_i|u_{l+1}\rangle]^{-\frac{1}{2}}$ 。综上, 由数学归纳法, 得原式成立, 证毕