课堂练习

练习1：对$S_{1/2}$空间和$L_2[0,a]$空间，分别写出其代表性右矢对应的左矢

解：对$S_{1/2}$空间，其代表性右矢为$|a\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$，对应的左矢为$\langle a| = \begin{bmatrix} a_1^* & a_2^* \end{bmatrix}$，为原矩阵的厄米共轭矩阵。
对$L_2[0,a]$空间，其代表性右矢为$|\varphi\rangle = \varphi(x)$，对应的左矢为$\langle\varphi| = \varphi^*(x)$，为原函数的复共轭函数。

练习2：设$\hat{B},\hat{C}$为可逆算符，证明$(\hat{B}\hat{C})^{-1} = \hat{C}^{-1}\hat{B}^{-1}$

证明：设$\hat{A} = \hat{B}\hat{C}$，则由于$\hat{B},\hat{C}$为可逆算符，故$\hat{A}$也为可逆算符，且有$\hat{A}^{-1}\hat{A} = \hat{I}$，代入得$(\hat{B}\hat{C})^{-1}\hat{B}\hat{C} = \hat{I}$，两边右乘$\hat{C}^{-1}\hat{B}^{-1}$，得:

$$\begin{aligned}\hat{C}^{-1}\hat{B}^{-1} &= (\hat{B}\hat{C})^{-1}\hat{B}\hat{C}\hat{C}^{-1}\hat{B}^{-1} = (\hat{B}\hat{C})^{-1}\hat{B}(\hat{C}\hat{C}^{-1})\hat{B}^{-1} = (\hat{B}\hat{C})^{-1}\hat{B}\hat{I}\hat{B}^{-1} \\ &= (\hat{B}\hat{C})^{-1}\hat{B}\hat{B}^{-1} = (\hat{B}\hat{C})^{-1}(\hat{B}\hat{B}^{-1}) = (\hat{B}\hat{C})^{-1}\end{aligned}$$

故原题得证。

练习3：对于任意矢量$|u\rangle, |v\rangle$均有$\langle u|\hat{A}|v\rangle = \langle u|\hat{B}|v\rangle$，则$\hat{A} = \hat{B}$

证明：移项可得$\langle u|(\hat{A}-\hat{B})|v\rangle = 0$，将$\langle u|$按共轭空间的基矢$\{\langle a_i|\}$展开，得$\langle u| = \sum\limits_i \langle u|a_i\rangle\langle a_i|$，从而有$\sum\limits_i \langle u|a_i\rangle\langle a_i|(\hat{A}-\hat{B})|v\rangle = 0$，该式对任意$|u\rangle, |v\rangle$均成立（因此可以取一个向量$|u\rangle$，使得对任意的$i$都有$\langle u|a_i\rangle \neq 0$），这意味着$(\hat{A}-\hat{B})|v\rangle$与共轭空间的所有基矢均正交，从而$(\hat{A}-\hat{B})|v\rangle$只能为零向量（否则$\langle u|(\hat{A}-\hat{B})|v\rangle = 0$不成立），即$|(\hat{A}-\hat{B})|v\rangle = \mathbf{0}$，移项得$\hat{A}|v\rangle = \hat{B}|v\rangle$，因此$\hat{A} = \hat{B}$，证毕

另证：原式两边左乘任意不为零的矢量$|w\rangle$，得$|w\rangle\langle u|\hat{A}|v\rangle = |w\rangle\langle u|\hat{B}|v\rangle$，即$(|w\rangle\langle u|\hat{A})\cdot|v\rangle = (|w\rangle\langle u|\hat{B})\cdot|v\rangle$。根据算符相等的定义，有$|w\rangle\langle u|\hat{A} = |w\rangle\langle u|\hat{B}$，然后再左乘相应的共轭矢量$\langle w|$，得$\langle w|w\rangle\langle u|\hat{A} = \langle w|w\rangle\langle u|\hat{B}$，消去$\langle w|w\rangle$得$\langle u|\hat{A} = \langle u|\hat{B}$，再根据算符相等的定义，得$\hat{A} = \hat{B}$

练习4：证明$(\hat{A}^\dagger)^\dagger = \hat{A}$

证明：对于矢量$|u\rangle, |v\rangle$，由算符的厄米共轭性质，得$\langle u|\hat{A}|v\rangle = \langle v|\hat{A}^\dagger|u\rangle^*$，两边取复共轭，得$\langle u|\hat{A}|v\rangle^* = \langle v|\hat{A}^\dagger|u\rangle$，另一方面，按照厄米共轭算符的定义，$\langle v|\hat{A}^\dagger|u\rangle = \langle u|(\hat{A}^\dagger)^\dagger|v\rangle^*$，因此$\langle u|\hat{A}|v\rangle^* = \langle u|(\hat{A}^\dagger)^\dagger|v\rangle^*$，两边再取复共轭，得$\langle u|\hat{A}|v\rangle = \langle u|(\hat{A}^\dagger)^\dagger|v\rangle$，结合前面的练习3，可得$(\hat{A}^\dagger)^\dagger = \hat{A}$。

练习5：试证明，如果对任意矢量$|u\rangle$，$\langle u|\hat{A}|u\rangle$都为实数，则算符$\hat{A}$为厄米算符

证明：因$\langle u|\hat{A}|u\rangle$为实数，故有$\langle u|\hat{A}|u\rangle = \langle u|\hat{A}|u\rangle^*$。又根据厄米共轭算符的定义，得$\langle u|\hat{A}|u\rangle^* = \langle u|\hat{A}^\dagger|u\rangle$，故有$\langle u|\hat{A}|u\rangle = \langle u|\hat{A}^\dagger|u\rangle$，根据练习3，可得$\hat{A} = \hat{A}^\dagger$，即算符$\hat{A}$为厄米算符

练习6：试证明，如果对任意矢量$|u\rangle$，$\langle u|\hat{A}^\dagger\hat{A}|u\rangle = \langle u|u\rangle$，则算符$\hat{A}$为幺正算符

证明：设有任意矢量$|u\rangle, |v\rangle$，它们的其中一种线性组合为$|w\rangle = |u\rangle + \lambda|v\rangle$，其中$\lambda$为非零复数，对应共轭矢量为$\langle w| = \langle u| + \lambda^*\langle v|$，则:

$$\langle w|w\rangle = (\langle u| + \lambda^*\langle v|)(|u\rangle + \lambda|v\rangle) = \langle u|u\rangle + \lambda\langle u|v\rangle + \lambda^*\langle v|u\rangle + \lambda\lambda^*\langle v|v\rangle$$

另一方面，用算符$\hat{A}$对前述线性组合进行变换，得$\hat{A}|w\rangle = \hat{A}|u\rangle + \lambda\hat{A}|v\rangle$（根据分配律和数乘交换律），其对应的共轭矢量为$\langle w|\hat{A}^\dagger = \langle u|\hat{A}^\dagger + \lambda^*\langle v|\hat{A}^\dagger$，因此:

$\langle w|\hat{A}^\dagger\hat{A}|w\rangle = (\langle u|\hat{A}^\dagger + \lambda^*\langle v|\hat{A}^\dagger)(\hat{A}|u\rangle + \lambda\hat{A}|v\rangle) = \langle u|\hat{A}^\dagger\hat{A}|u\rangle + \lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle + \lambda^*\langle v|\hat{A}^\dagger\hat{A}|u\rangle + \lambda\lambda^*\langle v|\hat{A}^\dagger\hat{A}|v\rangle$

结合题意，有 $\langle u|\hat{A}^\dagger\hat{A}|u\rangle = \langle u|u\rangle$ ， $\langle v|\hat{A}^\dagger\hat{A}|v\rangle = \langle v|v\rangle$ ， $\langle w|\hat{A}^\dagger\hat{A}|w\rangle = \langle w|w\rangle$，故联立并化简得：

$$\lambda\langle u|v\rangle + \lambda^*\langle v|u\rangle = \lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle + \lambda^*\langle v|\hat{A}^\dagger\hat{A}|u\rangle$$

又根据内积的性质，得$\langle u|v\rangle^* = \langle v|u\rangle$，再根据厄米共轭算符的定义，得$\langle u|\hat{A}^\dagger\hat{A}|v\rangle^* = \langle v|\hat{A}^\dagger\hat{A}|u\rangle$，因此有：

$$\begin{aligned}&\lambda\langle u|v\rangle + \lambda^*\langle u|v\rangle^* = \lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle + \lambda^*\langle u|\hat{A}^\dagger\hat{A}|v\rangle^*\\ \Rightarrow&\lambda\langle u|v\rangle + (\lambda\langle u|v\rangle)^* = \lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle + (\lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle)^*\\ \Rightarrow&2\Re(\lambda\langle u|v\rangle) = 2\Re(\lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle)\\ \Rightarrow&\Re(\lambda\langle u|v\rangle) = \Re(\lambda\langle u|\hat{A}^\dagger\hat{A}|v\rangle)\end{aligned}$$

取$\lambda = 1$，则有$\Re(\langle u|v\rangle) = \Re(\langle u|\hat{A}^\dagger\hat{A}|v\rangle)$；取$\lambda = -\mathrm{i}$，则有$\Re(-\mathrm{i}\langle u|v\rangle) = \Re(-\mathrm{i}\langle u|\hat{A}^\dagger\hat{A}|v\rangle)$，即$\Im(\langle u|v\rangle) = \Im(\langle u|\hat{A}^\dagger\hat{A}|v\rangle)$。从而得 $\langle u|\hat{A}^\dagger\hat{A}|v\rangle = \langle u|v\rangle = \langle u|\hat{I}|v\rangle$，根据练习3，得$\hat{A}^\dagger\hat{A} = \hat{I}$，即算符$\hat{A}$为幺正算符

练习7：在函数空间中，$\hat{d}_x$作用在右矢的定义是非常明确的，$\hat{d}_x|u\rangle = \frac{d}{dx}u(x)$。但根据前面的讨论，算符$\hat{d}_x$也应该能作用于左矢，那么如何定义$\langle u|\hat{d}_x$？

解：我们知道，$\frac{d}{dx}$是一个右结合的运算符，即波函数在坐标表象下表示时，形式上$\frac{d}{dx}$只能作用在其右侧的波函数$v(x)$，而不能作用在左侧的波函数$u(x)$，因此考虑函数空间的如下内积$\langle u|\hat{d}_x|v\rangle$，有：

$$\begin{aligned}\langle u|\hat{d}_x|v\rangle &= \int_0^a u^*(x)\hat{d}_x v(x)dx = \int_0^a u^*(x)\frac{dv(x)}{dx}dx = \int_0^a u^*(x)dv(x)\\ &= [u^*(x)v(x)]_0^a - \int_0^a du^*(x)v(x) \quad \text{（利用分部积分法）}\\ &= -\int_0^a du^*(x)v(x) \quad \text{（利用波函数的边界条件，即波函数在边界的函数值为0）}\end{aligned}$$

比较$\int_0^a u^*(x)\hat{d}_x v(x)dx$和$-\int_0^a du^*(x)v(x)$得$\langle u|\hat{d}_x = -\frac{d}{dx}u^*(x)$

练习8：在$L_2[0,a]$空间中证明：（1）$\hat{p}_x$是个厄米算符；（2）$\hat{p}_x$与x不对易，且满足$[\hat{x},\hat{p}_x] = \mathrm{i}\hbar$

证明：（1）易知：

$$\begin{aligned}\langle u|\hat{p}_x|v\rangle &= \int_0^a u^*(x)\hat{p}_x v(x)dx = \int_0^a u^*(x)[-\mathrm{i}\hbar\frac{dv(x)}{dx}]dx = -\mathrm{i}\hbar\int_0^a u^*(x)dv(x)\\ &= -\mathrm{i}\hbar\{[u^*(x)v(x)]_0^a - \int_0^a du^*(x)v(x)\} = -\mathrm{i}\hbar\{-\int_0^a du^*(x)v(x)\}\\ &= \int_0^a [\mathrm{i}\hbar\frac{du^*(x)}{dx}]v(x)dx = \int_0^a [\hat{p}_x u(x)]^* v(x)dx\\ &= [\int_0^a v^*(x)\hat{p}_x u(x)dx]^* = \langle v|\hat{p}_x|u\rangle^*\end{aligned}$$

因此根据定义，得$\hat{p}_x$是个厄米算符

（2）易知：

$$\begin{aligned}\langle u|\hat{x}\hat{p}_x|v\rangle &= \int_0^a u^*(x)\hat{x}\hat{p}_x v(x)dx = \int_0^a u^*(x)\hat{x}[-\mathrm{i}\hbar\frac{dv(x)}{dx}]dx = -\mathrm{i}\hbar\int_0^a u^*(x)\hat{x}dv(x)\\ &= -\mathrm{i}\hbar\int_0^a u^*(x)xdv(x) = -\mathrm{i}\hbar\int_0^a xu^*(x)dv(x)\end{aligned}$$

$$\begin{aligned}\langle u|\hat{p}_x\hat{x}|v\rangle &= \int_0^a u^*(x)\hat{p}_x\hat{x}v(x)dx = \int_0^a u^*(x)\hat{p}_x[xv(x)]dx = \int_0^a u^*(x)\{-\mathrm{i}\hbar\frac{d[xv(x)]}{dx}\}dx \\ &= -\mathrm{i}\hbar\int_0^a u^*(x)\{v(x)+\frac{dv(x)}{dx}\}dx = -\mathrm{i}\hbar\int_0^a u^*(x)\{v(x)+\frac{dv(x)}{dx}\}dx \\ &= -\mathrm{i}\hbar\int_0^a u^*(x)v(x)dx - \mathrm{i}\hbar\int_0^a xu^*(x)dv(x)\end{aligned}$$

因此：

$$\begin{aligned}\langle u|[\hat{x},\hat{p}_x]|v\rangle &= \langle u|(\hat{x}\hat{p}_x-\hat{p}_x\hat{x})|v\rangle = \langle u|\hat{x}\hat{p}_x|v\rangle - \langle u|\hat{p}_x\hat{x}|v\rangle = \mathrm{i}\hbar\int_0^a u^*(x)v(x)dx \\ &= \mathrm{i}\hbar\langle u|v\rangle = \langle u|(\mathrm{i}\hbar\hat{I})|v\rangle\end{aligned}$$

从而$[\hat{x},\hat{p}_x]=\mathrm{i}\hbar\hat{I}=\mathrm{i}\hbar$，证毕

练习9：试说明$\hat{x}\hat{p}_x$是否为厄米算符

解：易知：

$$\begin{aligned}\langle u|\hat{x}\hat{p}_x|v\rangle &= \int_0^a u^*(x)\hat{x}\hat{p}_x v(x)dx = \int_0^a u^*(x)\hat{x}[-\mathrm{i}\hbar\frac{dv(x)}{dx}]dx = -\mathrm{i}\hbar\int_0^a u^*(x)\hat{x}dv(x) \\ &= -\mathrm{i}\hbar\int_0^a u^*(x)xdv(x) = -\mathrm{i}\hbar\int_0^a xu^*(x)dv(x)\end{aligned}$$

$$\begin{aligned}\langle v|\hat{x}\hat{p}_x|u\rangle^* &= \Big[\int_0^a v^*(x)\hat{x}\hat{p}_x u(x)dx\Big]^* = \Big\{\int_0^a v^*(x)\hat{x}[-\mathrm{i}\hbar\frac{du(x)}{dx}]dx\Big\}^* = \Big\{-\mathrm{i}\hbar\int_0^a v^*(x)\hat{x}du(x)\Big\}^* \\ &= \Big\{-\mathrm{i}\hbar\int_0^a v^*(x)xdu(x)\Big\}^* = \mathrm{i}\hbar\int_0^a xv(x)du^*(x) = \mathrm{i}\hbar\Big\{[xv(x)u^*(x)]_0^a - \int_0^a u^*(x)d[xv(x)]\Big\} \\ &= \mathrm{i}\hbar\Big\{0-\int_0^a u^*(x)[v(x)dx+xdv(x)]\Big\} = -\mathrm{i}\hbar\int_0^a u^*(x)v(x)dx - \mathrm{i}\hbar\int_0^a xu^*(x)dv(x) \\ &= -\mathrm{i}\hbar\int_0^a u^*(x)v(x)dx + \langle u|\hat{x}\hat{p}_x|v\rangle \neq \langle u|\hat{x}\hat{p}_x|v\rangle\end{aligned}$$

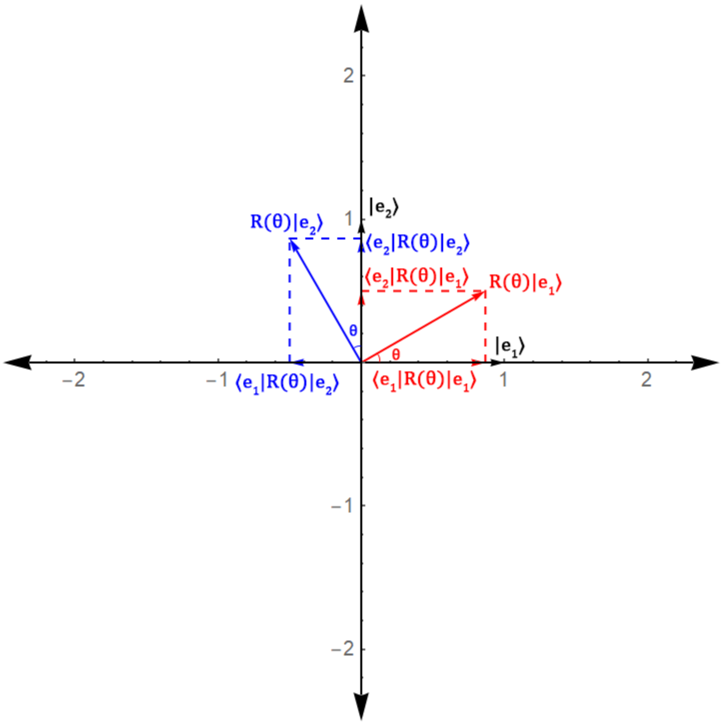
从而$\hat{x}\hat{p}_x$不是厄米算符，事实上，根据$\hat{p}_x$与x不对易，也能推测出$\hat{x}\hat{p}_x$不是厄米算符

练习10：推导(x,y)平面内旋转操作的表达式$\hat{R}(\theta)=\begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}$

解：(x,y)平面的基矢有两个：x轴方向的$|e_1\rangle$和y轴方向的$|e_2\rangle$，它们相互正交。因此，(x,y)平面的基矢经旋转操作$\hat{R}(\theta)$（即逆时针旋转θ度）后，将变换为$\hat{R}(\theta)|e_1\rangle$和$\hat{R}(\theta)|e_2\rangle$，而旋转操作的矩阵元分别为：

$$\langle e_1|\hat{R}(\theta)|e_1\rangle=\cos\theta \quad \langle e_2|\hat{R}(\theta)|e_1\rangle=\sin\theta \quad \langle e_1|\hat{R}(\theta)|e_2\rangle=-\sin\theta \quad \langle e_2|\hat{R}(\theta)|e_2\rangle=\cos\theta$$

因此有$\hat{R}(\theta)=\begin{bmatrix}\langle e_1|\hat{R}(\theta)|e_1\rangle & \langle e_1|\hat{R}(\theta)|e_2\rangle \\ \langle e_2|\hat{R}(\theta)|e_1\rangle & \langle e_2|\hat{R}(\theta)|e_2\rangle\end{bmatrix}=\begin{bmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{bmatrix}$，其几何关系如图所示：



练习11：证明如果一个厄米算符在一组正交归一的完备基矢上的表示是一个对角化的矩阵，则该基组中每个矢量也是该算符的本征矢，对角元即为相应的本征值

证明：根据题意，存在这样一个厄米算符$\hat{A}$，在正交归一的完备基矢$\{|a_i\rangle\}$ $(i=1,2,\dots,n)$的表示为

$\mathbf{A}=\begin{bmatrix} a_1 & 0 & \dots & 0 \\ 0 & a_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_n \end{bmatrix}$，即厄米算符$\hat{A}$对应的矩阵的元素满足$\langle a_i|\hat{A}|a_j\rangle = a_i\delta_{ij} = a_j\delta_{ij}$。

两边左乘$|a_i\rangle$，得$|a_i\rangle\langle a_i|\hat{A}|a_j\rangle = a_j\delta_{ij}|a_i\rangle$，再按$i$求和得$\sum\limits_{i=1}^{n}|a_i\rangle\langle a_i|\hat{A}|a_j\rangle = \sum\limits_{i=1}^{n}a_j\delta_{ij}|a_i\rangle$，其中：

$$\sum_{i=1}^{n}|a_i\rangle\langle a_i|\hat{A}|a_j\rangle = (\sum_{i=1}^{n}|a_i\rangle\langle a_i|)\cdot(\hat{A}|a_j\rangle) = \hat{I}\,\hat{A}|a_j\rangle = \hat{A}|a_j\rangle \quad \sum_{i=1}^{n}a_j\delta_{ij}|a_i\rangle = a_j|a_j\rangle$$

因此对任意的j，均有$\hat{A}|a_j\rangle = a_j|a_j\rangle$，证毕

练习12：已知$|b_i\rangle = \hat{U}|a_i\rangle$ $(i=1,2,\dots,n)$，其中$\{|a_i\rangle\}$和$\{|b_i\rangle\}$均为正交归一的完备基矢，能否写出算符$\hat{U}$的表达式？

解：原式两边右乘$\langle a_i|$，得$|b_i\rangle\langle a_i| = \hat{U}|a_i\rangle\langle a_i|$，再按$i$求和得

$\sum\limits_{i=1}^{n}|b_i\rangle\langle a_i| = \sum\limits_{i=1}^{n}\hat{U}|a_i\rangle\langle a_i| = \hat{U}\sum\limits_{i=1}^{n}|a_i\rangle\langle a_i| = \hat{U}\hat{I} = \hat{U}$，因此算符$\hat{U}$的表达式可写作$\hat{U} = \sum\limits_{i=1}^{n}|b_i\rangle\langle a_i|$

练习13：证明幺正算符对应的矩阵为幺正矩阵

证明：将幺正算符$\hat{U}$和相应的厄米共轭算符$\hat{U}^\dagger$在正交归一的完备基组$\{|a_i\rangle\}$展开，得：

$$\mathbf{U}=\begin{bmatrix} \langle a_1|\hat{U}|a_1\rangle & \langle a_1|\hat{U}|a_2\rangle & \dots & \langle a_1|\hat{U}|a_n\rangle \\ \langle a_2|\hat{U}|a_1\rangle & \langle a_2|\hat{U}|a_2\rangle & \dots & \langle a_2|\hat{U}|a_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle a_n|\hat{U}|a_1\rangle & \langle a_n|\hat{U}|a_2\rangle & \dots & \langle a_n|\hat{U}|a_n\rangle \end{bmatrix} \quad \mathbf{U}^\dagger=\begin{bmatrix} \langle a_1|\hat{U}^\dagger|a_1\rangle & \langle a_1|\hat{U}^\dagger|a_2\rangle & \dots & \langle a_1|\hat{U}^\dagger|a_n\rangle \\ \langle a_2|\hat{U}^\dagger|a_1\rangle & \langle a_2|\hat{U}^\dagger|a_2\rangle & \dots & \langle a_2|\hat{U}^\dagger|a_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle a_n|\hat{U}^\dagger|a_1\rangle & \langle a_n|\hat{U}^\dagger|a_2\rangle & \dots & \langle a_n|\hat{U}^\dagger|a_n\rangle \end{bmatrix}$$

将矩阵$\mathbf{U}$与$\mathbf{U}^\dagger$相乘，可得矩阵$\mathbf{U}\mathbf{U}^\dagger$的元素为：

$$(\mathbf{U}\mathbf{U}^\dagger)_{ij}=\sum_{k=1}^{n}\langle a_i|\hat{U}|a_k\rangle\langle a_k|\hat{U}^\dagger|a_j\rangle=\sum_{k=1}^{n}\left[(\langle a_i|\hat{U})\cdot(|a_k\rangle\langle a_k|)\cdot(\hat{U}^\dagger|a_j\rangle)\right]=(\langle a_i|\hat{U})\cdot(\sum_{k=1}^{n}|a_k\rangle\langle a_k|)\cdot(\hat{U}^\dagger|a_j\rangle)$$
$$=(\langle a_i|\hat{U})\cdot\hat{I}\cdot(\hat{U}^\dagger|a_j\rangle)=(\langle a_i|\hat{U})\cdot(\hat{U}^\dagger|a_j\rangle)=\langle a_i|\hat{U}\hat{U}^\dagger|a_j\rangle=\langle a_i|a_j\rangle=\delta_{ij}\quad\text{（利用算符的幺正性）}$$

矩阵$\mathbf{U}^\dagger\mathbf{U}$的元素为：

$$(\mathbf{U}^\dagger\mathbf{U})_{ij}=\sum_{k=1}^{n}\langle a_i|\hat{U}^\dagger|a_k\rangle\langle a_k|\hat{U}|a_j\rangle=\sum_{k=1}^{n}\left[(\langle a_i|\hat{U}^\dagger)\cdot(|a_k\rangle\langle a_k|)\cdot(\hat{U}|a_j\rangle)\right]=(\langle a_i|\hat{U}^\dagger)\cdot(\sum_{k=1}^{n}|a_k\rangle\langle a_k|)\cdot(\hat{U}|a_j\rangle)$$
$$=(\langle a_i|\hat{U}^\dagger)\cdot\hat{I}\cdot(\hat{U}|a_j\rangle)=(\langle a_i|\hat{U}^\dagger)\cdot(\hat{U}|a_j\rangle)=\langle a_i|\hat{U}^\dagger\hat{U}|a_j\rangle=\langle a_i|a_j\rangle=\delta_{ij}\quad\text{（利用算符的幺正性）}$$

因此$\mathbf{U}\mathbf{U}^\dagger=\mathbf{U}^\dagger\mathbf{U}=\mathbf{I}$，从而$\mathbf{U}^\dagger=\mathbf{U}^{-1}$，即$\mathbf{U}$是幺正矩阵

练习14：证明幺正变换算符$\hat{U}$在新、旧基组上的矩阵表示是一样的，均为

$$\hat{U}=\begin{bmatrix}\langle a_1|b_1\rangle & \langle a_1|b_2\rangle & \cdots\\ \langle a_2|b_1\rangle & \langle a_2|b_2\rangle & \cdots\\ \vdots & \vdots & \ddots\end{bmatrix}$$

证明：按定义，幺正变换算符$\hat{U}=\sum\limits_{i=1}^{n}|b_i\rangle\langle a_i|$，因此对于旧基组$\{|a_i\rangle\}$，有：

$$\langle a_i|\hat{U}|a_j\rangle=\langle a_i|\cdot(\sum_{k=1}^{n}|b_k\rangle\langle a_k|)\cdot|a_j\rangle=\langle a_i|\cdot(\sum_{k=1}^{n}|b_k\rangle\langle a_k|a_j\rangle)=\langle a_i|\cdot(\sum_{k=1}^{n}|b_k\rangle\delta_{kj})=\langle a_i|\cdot|b_j\rangle=\langle a_i|b_j\rangle$$

对于新基组$\{|b_i\rangle\}$，有：

$$\langle b_i|\hat{U}|b_j\rangle=\langle b_i|\cdot(\sum_{k=1}^{n}|b_k\rangle\langle a_k|)\cdot|b_j\rangle=(\sum_{k=1}^{n}\langle b_i|b_k\rangle\langle a_k|)\cdot|b_j\rangle=(\sum_{k=1}^{n}\delta_{ik}\langle a_k|)\cdot|b_j\rangle=\langle a_i|\cdot|b_j\rangle=\langle a_i|b_j\rangle$$

因此幺正变换算符$\hat{U}$在新、旧基组上的矩阵表示是一样的，其矩阵元素均为$\langle a_i|b_j\rangle$，相应的矩阵表示与题述一致，证毕

练习15：求$Tr(|a_i\rangle\langle a_j|)=?$，$Tr(|a_i\rangle\langle b_j|)=?$，这里$\{|a_i\rangle\}$和$\{|b_i\rangle\}$分别是同一空间的两组完备的正交归一化基矢

解：根据算符的迹的定义，得：

$$Tr(|a_i\rangle\langle a_j|)=\sum_k\langle a_k|\cdot(|a_i\rangle\langle a_j|)\cdot|a_k\rangle=\sum_k\langle a_k|a_i\rangle\langle a_j|a_k\rangle=\langle a_i|a_i\rangle\langle a_j|a_i\rangle=1\cdot\delta_{ji}=\delta_{ji}$$

$$Tr(|a_i\rangle\langle b_j|)=\sum_k\langle a_k|\cdot(|a_i\rangle\langle b_j|)\cdot|a_k\rangle=\sum_k\langle a_k|a_i\rangle\langle b_j|a_k\rangle=\langle a_i|a_i\rangle\langle b_j|a_i\rangle=1\cdot\langle b_j|a_i\rangle=\langle b_j|a_i\rangle$$

练习16：写出$f(\hat{A})$作用在任意矢量$|u\rangle$上的计算表达式

解：将$|u\rangle$在$\hat{A}$的正交归一的完备基组$\{|a_i\rangle\}$上展开，得$|u\rangle=\sum\limits_i u_{a_i}|a_i\rangle$，将$f(\hat{A})$作用在矢量$|u\rangle$上，可得：

$$f(\hat{A})|u\rangle=f(\hat{A})(\sum_i u_{a_i}|a_i\rangle)=\sum_i u_{a_i}f(\hat{A})|a_i\rangle=\sum_i u_{a_i}f(a_i)|a_i\rangle$$

练习17：证明Baker-Hausdorff公式

证明：根据$\mathrm{e}^{\hat{A}}$和$\mathrm{e}^{-\hat{A}}$的展开式（此处定义$\hat{A}^0=\hat{I}$）

$$\mathrm{e}^{\hat{A}}=\sum_{i=0}^{\infty}\frac{1}{i!}\hat{A}^i\quad \mathrm{e}^{-\hat{A}}=\sum_{i=0}^{\infty}\frac{(-1)^i}{i!}\hat{A}^i$$

以上公式可改写为：

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}=(\sum_{i=0}^{\infty}\frac{1}{i!}\hat{A}^{i})\hat{B}\Big[\sum_{j=0}^{\infty}\frac{(-1)^{j}}{j!}\hat{A}^{j}\Big]=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\frac{(-1)^{j}}{i!j!}\hat{A}^{i}\hat{B}\hat{A}^{j}=\sum_{k=0}^{\infty}\sum_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}\quad(\text{令}k=i+j)$$

对比上式与贝克-豪斯多夫公式，我们可以猜想$\sum\limits_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}=\frac{1}{k!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{k\text{层对易符号}}$，特别的，当k=0时，右式变为$\hat{B}$，现在采用数学归纳法予以证明。

$k=0$时，左式为$\frac{(-1)^{0}}{0!0!}\hat{A}^{0}\hat{B}\hat{A}^{0}=\hat{I}\hat{B}\hat{I}=\frac{1}{0!}\hat{B}$；$k=1$时，左式为$\frac{(-1)^{1}}{0!1!}\hat{A}^{0}\hat{B}\hat{A}^{1}+\frac{(-1)^{0}}{1!0!}\hat{A}^{1}\hat{B}\hat{A}^{0}=-\hat{I}\hat{B}\hat{A}+\hat{A}\hat{B}\hat{I}=\frac{1}{1!}[\hat{A},\hat{B}]$。两者均符合题意。设$k=n$时，原猜想成立，则$k=n+1$时，有：

$$\begin{aligned}
\sum_{i=0}^{n+1}\frac{(-1)^{n+1-i}}{i!(n+1-i)!}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}&=\sum_{i=0}^{n+1}\frac{(-1)^{n+1-i}}{(n+1)!}\mathrm{C}_{n+1}^{i}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}=\sum_{i=0}^{n+1}\frac{(-1)^{n+1-i}}{(n+1)!}(\mathrm{C}_{n}^{i}+\mathrm{C}_{n}^{i-1})\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}\quad(\text{根据组合数性质})\\
&=\sum_{i=0}^{n}\frac{(-1)^{n+1-i}}{(n+1)!}\mathrm{C}_{n}^{i}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}+\sum_{i=1}^{n+1}\frac{(-1)^{n+1-i}}{(n+1)!}\mathrm{C}_{n}^{i-1}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}\\
&=\sum_{i=0}^{n}\frac{(-1)^{n+1-i}}{i!(n-i)!(n+1)}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}+\sum_{i=1}^{n+1}\frac{(-1)^{n+1-i}}{(i-1)!(n-i+1)!(n+1)}\hat{A}^{i}\hat{B}\hat{A}^{n+1-i}\\
&=\frac{1}{n+1}\Big\{-\Big[\sum_{i=0}^{n}\frac{(-1)^{n-i}}{i!(n-i)!}\hat{A}^{i}\hat{B}\hat{A}^{n-i}\Big]\hat{A}+\hat{A}\Big[\sum_{i'=0}^{n}\frac{(-1)^{n-i'}}{i'!(n-i')!}\hat{A}^{i'}\hat{B}\hat{A}^{n-i'}\Big]\Big\}\\
&=\frac{1}{n+1}\{-\frac{1}{n!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{n\text{层对易符号}}\cdot\hat{A}+\hat{A}\cdot\frac{1}{n!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{n\text{层对易符号}}\}\\
&=\frac{1}{n+1}\frac{1}{n!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{(n+1)\text{层对易符号}}=\frac{1}{(n+1)!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{(n+1)\text{层对易符号}}
\end{aligned}$$

因此根据数学归纳法，得猜想$\sum\limits_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}=\frac{1}{k!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{k\text{层对易符号}}$成立，从而有：

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}=\sum_{k=0}^{\infty}\sum_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}=\sum_{k=0}^{\infty}\frac{1}{k!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{k\text{层对易符号}}$$

故原题得证

练习18：设矩阵$\mathbf{A}=\begin{bmatrix}a&b\\b&a\end{bmatrix}$，证明对应于函数$f(x)$有（假定$f(x)$在$x=0$处的Taylor展开收敛）

$$f(\mathbf{A})=\begin{bmatrix}\frac{1}{2}[f(a+b)+f(a-b)]&\frac{1}{2}[f(a+b)-f(a-b)]\\\frac{1}{2}[f(a+b)-f(a-b)]&\frac{1}{2}[f(a+b)+f(a-b)]\end{bmatrix}$$

证明：将函数$f(x)$在$x=0$处作Taylor展开，得$f(x)=\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}x^{n}$，因此$f(a+b)=\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a+b)^{n}$，$f(a-b)=\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a-b)^{n}$；又根据函数作用在矩阵的定义，有$f(\mathbf{A})=\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\mathbf{A}^{n}$，现在我们要求$\mathbf{A}^{n}$。

作为特殊条件，当$n=0$时，我们定义$\mathbf{A}^{0}=\mathbf{I}$；当$n=1$时，我们有$\mathbf{A}^{1}=\mathbf{A}$；当$n=2,3,4$时，展开可得：

$$
\mathbf{A}^2=\mathbf{A}\cdot\mathbf{A}=\begin{bmatrix} a & b\\ b & a\end{bmatrix}\cdot\begin{bmatrix} a & b\\ b & a\end{bmatrix}=\begin{bmatrix} a^2+b^2 & 2ab\\ 2ab & a^2+b^2\end{bmatrix}
$$
$$
\mathbf{A}^3=\mathbf{A}\cdot\mathbf{A}^2=\begin{bmatrix} a & b\\ b & a\end{bmatrix}\cdot\begin{bmatrix} a^2+b^2 & 2ab\\ 2ab & a^2+b^2\end{bmatrix}=\begin{bmatrix} a^3+3ab^2 & 3a^2b+b^3\\ 3a^2b+b^3 & a^3+3ab^2\end{bmatrix}
$$
$$
\mathbf{A}^4=\mathbf{A}\cdot\mathbf{A}^3=\begin{bmatrix} a & b\\ b & a\end{bmatrix}\cdot\begin{bmatrix} a^3+3ab^2 & 3a^2b+b^3\\ 3a^2b+b^3 & a^3+3ab^2\end{bmatrix}=\begin{bmatrix} a^4+6a^2b^2+b^4 & 4a^3b+4ab^3\\ 4a^3b+4ab^3 & a^4+6a^2b^2+b^4\end{bmatrix}
$$

因此我们猜测，$\mathbf{A}^n$满足$\mathbf{A}^n=\begin{bmatrix}\frac{1}{2}[(a+b)^n+(a-b)^n] & \frac{1}{2}[(a+b)^n-(a-b)^n]\\ \frac{1}{2}[(a+b)^n-(a-b)^n] & \frac{1}{2}[(a+b)^n+(a-b)^n]\end{bmatrix}$。现在用数学归纳法加以证明。
由前述可知，对于n较小的情形，上式均能成立。假设上式在$k=n$时成立，则$k=n+1$时，有：

$$
\begin{aligned}
\mathbf{A}^{n+1}=\mathbf{A}\cdot\mathbf{A}^n&=\begin{bmatrix} a & b\\ b & a\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{2}[(a+b)^n+(a-b)^n] & \frac{1}{2}[(a+b)^n-(a-b)^n]\\ \frac{1}{2}[(a+b)^n-(a-b)^n] & \frac{1}{2}[(a+b)^n+(a-b)^n]\end{bmatrix}\\
&=\begin{bmatrix}\frac{a}{2}[(a+b)^n+(a-b)^n]+\frac{b}{2}[(a+b)^n-(a-b)^n] & \frac{b}{2}[(a+b)^n+(a-b)^n]+\frac{a}{2}[(a+b)^n-(a-b)^n]\\ \frac{b}{2}[(a+b)^n+(a-b)^n]+\frac{a}{2}[(a+b)^n-(a-b)^n] & \frac{a}{2}[(a+b)^n+(a-b)^n]+\frac{b}{2}[(a+b)^n-(a-b)^n]\end{bmatrix}\\
&=\begin{bmatrix}\frac{a+b}{2}(a+b)^n+\frac{a-b}{2}(a-b)^n & \frac{a+b}{2}(a+b)^n+\frac{b-a}{2}(a-b)^n\\ \frac{a+b}{2}(a+b)^n+\frac{b-a}{2}(a-b)^n & \frac{a+b}{2}(a+b)^n+\frac{a-b}{2}(a-b)^n\end{bmatrix}\\
&=\begin{bmatrix}\frac{1}{2}[(a+b)^{n+1}+(a-b)^{n+1}] & \frac{1}{2}[(a+b)^{n+1}-(a-b)^{n+1}]\\ \frac{1}{2}[(a+b)^{n+1}-(a-b)^{n+1}] & \frac{1}{2}[(a+b)^{n+1}+(a-b)^{n+1}]\end{bmatrix}
\end{aligned}
$$

因此猜想得证，从而有：

$$
\begin{aligned}
f(\mathbf{A})=\sum_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\mathbf{A}^n&=\sum_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\begin{bmatrix}\frac{1}{2}[(a+b)^n+(a-b)^n] & \frac{1}{2}[(a+b)^n-(a-b)^n]\\ \frac{1}{2}[(a+b)^n-(a-b)^n] & \frac{1}{2}[(a+b)^n+(a-b)^n]\end{bmatrix}\\
&=\begin{bmatrix}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\{\frac{1}{2}[(a+b)^n+(a-b)^n]\} & \sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\{\frac{1}{2}[(a+b)^n-(a-b)^n]\}\\ \sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\{\frac{1}{2}[(a+b)^n-(a-b)^n]\} & \sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}\{\frac{1}{2}[(a+b)^n+(a-b)^n]\}\end{bmatrix}\\
&=\begin{bmatrix}\frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a+b)^n+\frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a-b)^n & \frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a+b)^n-\frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a-b)^n\\ \frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a+b)^n-\frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a-b)^n & \frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a+b)^n+\frac{1}{2}\sum\limits_{i=0}^{\infty}\frac{f^{(n)}(0)}{i!}(a-b)^n\end{bmatrix}\\
&=\begin{bmatrix}\frac{1}{2}f(a+b)+\frac{1}{2}f(a-b) & \frac{1}{2}f(a+b)-\frac{1}{2}f(a-b)\\ \frac{1}{2}f(a+b)-\frac{1}{2}f(a-b) & \frac{1}{2}f(a+b)+\frac{1}{2}f(a-b)\end{bmatrix}\\
&=\begin{bmatrix}\frac{1}{2}[f(a+b)+f(a-b)] & \frac{1}{2}[f(a+b)-f(a-b)]\\ \frac{1}{2}[f(a+b)-f(a-b)] & \frac{1}{2}[f(a+b)+f(a-b)]\end{bmatrix}
\end{aligned}
$$

故原命题得证

练习19：证明$[\Delta\hat{A},\Delta\hat{B}]=[\hat{A},\hat{B}]$

证明：因为

$$
\begin{aligned}
[\Delta\hat{A},\Delta\hat{B}]&=[\hat{A}-\langle\hat{A}\rangle,\hat{B}-\langle\hat{B}\rangle]=(\hat{A}-\langle\hat{A}\rangle)(\hat{B}-\langle\hat{B}\rangle)-(\hat{B}-\langle\hat{B}\rangle)(\hat{A}-\langle\hat{A}\rangle)\\
&=(\hat{A}\hat{B}-\langle\hat{A}\rangle\hat{B}-\langle\hat{B}\rangle\hat{A}+\langle\hat{A}\rangle\langle\hat{B}\rangle)-(\hat{B}\hat{A}-\langle\hat{B}\rangle\hat{A}-\langle\hat{A}\rangle\hat{B}+\langle\hat{B}\rangle\langle\hat{A}\rangle)\text{（}\langle\hat{A}\rangle,\langle\hat{B}\rangle\text{均为实数，满足与算符的交换律）}\\
&=\hat{A}\hat{B}-\langle\hat{A}\rangle\hat{B}-\langle\hat{B}\rangle\hat{A}+\langle\hat{A}\rangle\langle\hat{B}\rangle-\hat{B}\hat{A}+\langle\hat{B}\rangle\hat{A}+\langle\hat{A}\rangle\hat{B}-\langle\hat{B}\rangle\langle\hat{A}\rangle\\
&=\hat{A}\hat{B}-\hat{B}\hat{A}\text{（}\langle\hat{A}\rangle,\langle\hat{B}\rangle\text{均为实数，满足}\langle\hat{A}\rangle\langle\hat{B}\rangle=\langle\hat{B}\rangle\langle\hat{A}\rangle\text{）}\\
&=[\hat{A},\hat{B}]
\end{aligned}
$$

故原题得证

第一章习题

1.1 如果一个算符$\hat{A}$满足$\hat{A}^\dagger=-\hat{A}$，称之为反厄米的。证明反厄米算符最多只有一个实的本征值

证明：对于算符$\hat{A}$对应的正交归一的完备基组$\{|a_i\rangle\}$，有$\hat{A}|a_i\rangle=a_i|a_i\rangle$，两边左乘$\langle a_i|$得$\langle a_i|\hat{A}|a_i\rangle=a_i\langle a_i|a_i\rangle=a_i$，然后两边取共轭得$\langle a_i|\hat{A}|a_i\rangle^*=\langle a_i|\hat{A}^\dagger|a_i\rangle=a_i^*$。根据反厄米算符的性质，有$\hat{A}^\dagger=-\hat{A}$，因此$\langle a_i|\hat{A}^\dagger|a_i\rangle=\langle a_i|(-\hat{A})|a_i\rangle=-\langle a_i|\hat{A}|a_i\rangle=-a_i$，两者结合可以得知$a_i^*=-a_i$，即$a_i+a_i^*=2\Re a_i=0$，因此$\Re a_i=0$，这意味着$a_i$要么为纯虚数，要么为0，从而反厄米算符$\hat{A}$最多只有一个实的本征值，证毕

1.2 证明$\hat{A}\hat{B}-\hat{B}\hat{A}=\hat{I}$不可能在有限维的矩阵表示上成立，其中$\hat{I}$为单位算符。

证明：根据算符迹的性质，有$Tr(\hat{A}\hat{B})=Tr(\hat{B}\hat{A})$，且$Tr(\hat{A}\hat{B}-\hat{B}\hat{A})=Tr(\hat{A}\hat{B})-Tr(\hat{B}\hat{A})=0$，而对于$n$维空间，有$Tr(\hat{I})=n$，因此$Tr(\hat{A}\hat{B}-\hat{B}\hat{A})\neq Tr(\hat{I})$，从而无法找到合适的$\hat{A}\hat{B}-\hat{B}\hat{A}$，使得该算符的迹等于单位算符的迹，而算符的迹相等是算符相等的必要条件（算符相等可推出算符的迹相等，但算符的迹相等不能推出算符相等），因此$\hat{A}\hat{B}-\hat{B}\hat{A}=\hat{I}$不可能在有限维的矩阵表示上成立

1.3 考虑一个由正交归一矢$|1\rangle,|2\rangle$展开的二维矢量空间，算符为$\hat{H}=a(|1\rangle\langle 1|-|2\rangle\langle 2|+|1\rangle\langle 2|+|2\rangle\langle 1|)$，其中$a$为一实常数。求出$\hat{H}$的本征值和本征矢

解：设$\hat{H}$的本征矢为$|h_i\rangle\ (i=1,2)$，相应的本征值为$h_i\ (i=1,2)$，则由于：

$$\langle 1|\hat{H}|1\rangle=a\quad\langle 1|\hat{H}|2\rangle=a\quad\langle 2|\hat{H}|1\rangle=a\quad\langle 2|\hat{H}|2\rangle=-a$$

因此$\hat{H}$的矩阵表示为$\mathbf{H}=\begin{bmatrix}a & a\\ a & -a\end{bmatrix}$，从而可列出方程$\mathbf{H}\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=h_i\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}$（或写作$(\mathbf{H}-h_i\mathbf{I})\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=\mathbf{0}$）相应的久期方程为：

$$|\mathbf{H}-h_i\mathbf{I}|=\begin{vmatrix}a-h_i & a\\ a & -a-h_i\end{vmatrix}=(a-h_i)(-a-h_i)-a^2=0$$

解得$h_i=\pm\sqrt{2}a$。

当$h_i=\sqrt{2}a$时，代回方程$(\mathbf{H}-h_i\mathbf{I})\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=\mathbf{0}$，得$\begin{bmatrix}a-\sqrt{2}a & a\\ a & -a-\sqrt{2}a\end{bmatrix}\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=\mathbf{0}$，从而有$(a-\sqrt{2}a)\langle 1|h_i\rangle+a\langle 2|h_i\rangle=0$，即$\langle 2|h_i\rangle=(\sqrt{2}-1)\langle 1|h_i\rangle$，取$\langle 1|h_i\rangle=1$，则$\langle 2|h_i\rangle=\sqrt{2}-1$，因此$\hat{H}$的本征矢之一为$|h_1\rangle=k_1|1\rangle+(\sqrt{2}-1)k_1|2\rangle\ (k_1\neq 0)$；

当$h_i=-\sqrt{2}a$时，代回方程$(\mathbf{H}-h_i\mathbf{I})\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=\mathbf{0}$，得$\begin{bmatrix}a+\sqrt{2}a & a\\ a & -a+\sqrt{2}a\end{bmatrix}\begin{bmatrix}\langle 1|h_i\rangle\\ \langle 2|h_i\rangle\end{bmatrix}=\mathbf{0}$，从而有$(a+\sqrt{2}a)\langle 1|h_i\rangle+a\langle 2|h_i\rangle=0$，即$\langle 2|h_i\rangle=-(\sqrt{2}+1)\langle 1|h_i\rangle$，取$\langle 1|h_i\rangle=1$，则$\langle 2|h_i\rangle=-(\sqrt{2}+1)$，因此$\hat{H}$的本征矢之二为$|h_2\rangle=k_2|1\rangle-(\sqrt{2}+1)k_2|2\rangle\ (k_2\neq 0)$