课堂练习

练习1：证明$(\hat{A}^\dagger)^\dagger = \hat{A}$

证明：首先要证明如下引理：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$\hat{A} = \hat{B}$。以下是可能的证明思路：

证明1：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$\langle u| = \sum_i \langle u|a_i\rangle\langle a_i|$，从而有$\sum_i \langle u|a_i\rangle\langle a_i|(\hat{A}-\hat{B})|v\rangle = 0$，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

证明2：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$\hat{A} = \hat{B}$

现在回到本题。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$\langle u|\hat{A}|v\rangle = \langle u|(\hat{A}^\dagger)^\dagger|v\rangle$，结合前面的引理，可得$(\hat{A}^\dagger)^\dagger = \hat{A}$

练习2：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1的引理，可得$\hat{A} = \hat{A}^\dagger$，即算符$\hat{A}$为厄米算符

练习3：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1的引理，得$\hat{A}^\dagger\hat{A}=\hat{I}$，即算符$\hat{A}$为幺正算符

练习4：如果$\hat{A}|u\rangle=|v\rangle$，则显然有$\hat{A}|u\rangle=|v\rangle\langle u|u\rangle=(|v\rangle\langle u|)\cdot|u\rangle$（假定$|u\rangle$是个归一化矢量），是否由此可以得出$\hat{A}=|v\rangle\langle u|$?

解：算符相等的定义为：对于任意向量$|u\rangle$，均有$\hat{A}|u\rangle=\hat{B}|u\rangle$，则$\hat{A}=\hat{B}$。显然对于题述情形，由于仅仅存在$|u\rangle$，使得$\hat{A}|u\rangle=(|v\rangle\langle u|)\cdot|u\rangle$，因此并不能说明$\hat{A}=|v\rangle\langle u|$。事实上，取$\hat{A}=|v\rangle(\langle u|+\lambda\langle w|)=|v\rangle\langle u|+\lambda|v\rangle\langle w|$，其中λ为任意复数，$\langle w|$为满足$\langle w|u\rangle=0$的任意向量，则：

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

显然满足题意，但当$\lambda\neq 0$时，$\hat{A}\neq|v\rangle\langle u|$

练习5：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6：在$L_2[0,a]$空间中证明：$\hat{p}_x$是个厄米算符

证明：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

练习7：证明贝克-豪斯多夫公式

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}=\hat{B}+[\hat{A},\hat{B}]+\frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]+\frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]+\ldots$$

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：

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

对比上式与贝克-豪斯多夫公式，我们可以猜想$\sum_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}=\frac{1}{k!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{k\text{层对易符号}}$，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$\sum_{i=0}^{k}\frac{(-1)^{k-i}}{i!(k-i)!}\hat{A}^{i}\hat{B}\hat{A}^{k-i}=\frac{1}{k!}\underbrace{[\hat{A},[\ldots,[\hat{A},\hat{B}]]]}_{k\text{层对易符号}}$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8：证明$\widetilde{\langle a|}\cdot\widetilde{|a\rangle}=\mathbf{I}$（即$n\times n$的单位矩阵）

证明：易知$\widetilde{\langle a|}=\begin{bmatrix}\langle a_1|\\ \langle a_2|\\ \vdots\\ \langle a_n|\end{bmatrix}$，$\widetilde{|a\rangle}=[\,|a_1\rangle\quad|a_2\rangle\quad\ldots\quad|a_n\rangle\,]$，两个矩阵相乘，得：

$$\widetilde{\langle a|}\cdot\widetilde{|a\rangle}=\begin{bmatrix}\langle a_1|\\ \langle a_2|\\ \vdots\\ \langle a_n|\end{bmatrix}\begin{bmatrix}|a_1\rangle & |a_2\rangle & \dots & |a_n\rangle\end{bmatrix}=\begin{bmatrix}\langle a_1|a_1\rangle & \langle a_1|a_2\rangle & \dots & \langle a_1|a_n\rangle\\ \langle a_2|a_1\rangle & \langle a_2|a_2\rangle & \dots & \langle a_2|a_n\rangle\\ \vdots & \vdots & \ddots & \vdots\\ \langle a_n|a_1\rangle & \langle a_n|a_2\rangle & \dots & \langle a_n|a_n\rangle\end{bmatrix}$$
$$=\begin{bmatrix}\langle a_1|a_1\rangle & \langle a_1|a_2\rangle & \dots & \langle a_1|a_n\rangle\\ \langle a_2|a_1\rangle & \langle a_2|a_2\rangle & \dots & \langle a_2|a_n\rangle\\ \vdots & \vdots & \ddots & \vdots\\ \langle a_n|a_1\rangle & \langle a_n|a_2\rangle & \dots & \langle a_n|a_n\rangle\end{bmatrix}=\begin{bmatrix}\delta_{11} & \delta_{12} & \dots & \delta_{1n}\\ \delta_{21} & \delta_{22} & \dots & \delta_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ \delta_{n1} & \delta_{n2} & \dots & \delta_{nn}\end{bmatrix}$$
$$=\begin{bmatrix}1 & 0 & \dots & 0\\ 0 & 1 & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & 1\end{bmatrix}=\mathbf{I}$$

故原题得证

练习9：证明任意幺正算符$\hat{U}$的矩阵表示U是幺正矩阵

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：

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

矩阵$\mathbf{U}^\dagger\mathbf{U}$的元素为：

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

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10：证明基矢变换算符$\hat{U}=\sum\limits_i|b_i\rangle\langle a_i|$是幺正算符，即$\hat{U}^\dagger=\hat{U}^{-1}$

证明：首先写出基矢变换算符$\hat{U}$对应的厄米共轭算符$\hat{U}^\dagger=\sum\limits_i|a_i\rangle\langle b_i|$，则：

$$\hat{U}\hat{U}^\dagger=(\sum_i|b_i\rangle\langle a_i|)\cdot(\sum_j|a_j\rangle\langle b_j|)=\sum_i\sum_j|b_i\rangle\langle a_i|a_j\rangle\langle b_j|=\sum_i\sum_j\delta_{ij}|b_i\rangle\langle b_j|=\sum_i|b_i\rangle\langle b_i|=\hat{I}$$

$$\hat{U}^\dagger\hat{U}=(\sum_i|a_i\rangle\langle b_i|)\cdot(\sum_j|b_j\rangle\langle a_j|)=\sum_i\sum_j|a_i\rangle\langle b_i|b_j\rangle\langle a_j|=\sum_i\sum_j\delta_{ij}|a_i\rangle\langle a_j|=\sum_i|a_i\rangle\langle a_i|=\hat{I}$$

因此对第一个等式左乘$\hat{U}^{-1}$，或对第二个等式右乘$\hat{U}^{-1}$，均有$\hat{U}^\dagger=\hat{U}^{-1}$，即基矢变换算符$\hat{U}$是幺正算符

习题1.4

1.如何从$|b_i\rangle=\hat{U}|a_i\rangle$推导$\hat{U}=\sum\limits_i|b_i\rangle\langle a_i|$?

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$\hat{U}=\sum\limits_{i=1}^{n}|b_i\rangle\langle a_i|$

2.已知二维空间中的一组正交归一基矢$|i\rangle,|j\rangle$，以此为基组写出另外一组正交归一的基矢

解：由题意可知$\langle i|i\rangle=\langle j|j\rangle=1$，$\langle i|j\rangle=\langle j|i\rangle=0$，因此有：

$$\begin{cases}(\langle i|+\langle j|)(|i\rangle+|j\rangle)=\langle i|i\rangle+\langle i|j\rangle+\langle j|i\rangle+\langle j|j\rangle=2\\(\langle i|-\langle j|)(|i\rangle-|j\rangle)=\langle i|i\rangle-\langle i|j\rangle-\langle j|i\rangle+\langle j|j\rangle=2\\(\langle i|+\langle j|)(|i\rangle-|j\rangle)=\langle i|i\rangle-\langle i|j\rangle+\langle j|i\rangle-\langle j|j\rangle=0\\(\langle i|-\langle j|)(|i\rangle+|j\rangle)=\langle i|i\rangle+\langle i|j\rangle-\langle j|i\rangle-\langle j|j\rangle=0\end{cases}$$

从而$|i\rangle+|j\rangle$与$|i\rangle-|j\rangle$正交，设$|i^{'}\rangle=\frac{1}{\sqrt{2}}(|i\rangle+|j\rangle)$，$|j^{'}\rangle=\frac{1}{\sqrt{2}}(|i\rangle-|j\rangle)$，则由上式知：

$$\begin{cases}\langle i^{'}|i^{'}\rangle=\frac{1}{2}(\langle i|+\langle j|)(|i\rangle+|j\rangle)=\frac{1}{2}\times2=1\\\langle j^{'}|j^{'}\rangle=\frac{1}{2}(\langle i|-\langle j|)(|i\rangle-|j\rangle)=\frac{1}{2}\times2=1\\\langle i^{'}|j^{'}\rangle=\frac{1}{2}(\langle i|+\langle j|)(|i\rangle-|j\rangle)=\frac{1}{2}\times0=0\\\langle j^{'}|i^{'}\rangle=\frac{1}{2}(\langle i|-\langle j|)(|i\rangle+|j\rangle)=\frac{1}{2}\times0=0\end{cases}$$

故另外一组正交归一的基矢为$|i^{'}\rangle=\frac{1}{\sqrt{2}}(|i\rangle+|j\rangle)$，$|j^{'}\rangle=\frac{1}{\sqrt{2}}(|i\rangle-|j\rangle)$

3.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：

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

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