QM - Homework 1

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Problem1

(a)

已知

$$\begin{cases} \hat{K}\left|1\right\rangle = 2\left|1\right\rangle \\ \hat{K}\left|2\right\rangle = 3\left|2\right\rangle \\ \hat{K}\left|3\right\rangle = -6\left|3\right\rangle \end{cases}$$

则可将 $\hat{K}$ 用其本征值和本征矢表示为:

$$\hat{K} = 2\left|1\right\rangle\left\langle 1\right| + 3\left|2\right\rangle\left\langle 2\right| - 6\left|3\right\rangle\left\langle 3\right|$$

其中 $\left|n\right\rangle\left\langle n\right|$ 为投影算符。
同样的，可将 $\hat{K}$ 表示为一个对角矩阵，其对角元即为在 $\{\left|1\right\rangle, \left|2\right\rangle, \left|3\right\rangle\}$ 本征矢所对应的本征值：

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}$$

(b)

已知 $\left|\alpha\right\rangle = \frac{1}{4}(-3\left|1\right\rangle + i\sqrt{6}\left|2\right\rangle + \left|3\right\rangle)$，则有：

$$\begin{aligned}
\left\langle\alpha\right|\hat{K}\left|\alpha\right\rangle &= \frac{1}{4}\cdot\frac{1}{4}((-3)^\dagger\left\langle 1\right| + (i\sqrt{6})^\dagger\left\langle 2\right| + \left\langle 3\right|)\cdot\hat{K}\cdot(-3\left|1\right\rangle + i\sqrt{6}\left|2\right\rangle + \left|3\right\rangle) \\
&= \frac{1}{16}(9\left\langle 1\right|\hat{K}\left|1\right\rangle + 6\left\langle 2\right|\hat{K}\left|2\right\rangle + \left\langle 3\right|\hat{K}\left|3\right\rangle) \\
&= \frac{1}{16}(9\times 2\left\langle 1|1\right\rangle + 6\times 3\left\langle 2|2\right\rangle - 6\left\langle 3|3\right\rangle) \\
&= \frac{1}{16}(18 + 18 - 6) \\
&= \frac{15}{8}
\end{aligned}$$

Problem2

已知 $\hat{H} = a(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|)$ 则有

$$\hat{H}\begin{pmatrix}|1\rangle \\ |2\rangle\end{pmatrix} = \begin{pmatrix}a|1\rangle + a|2\rangle \\ a|1\rangle - a|2\rangle\end{pmatrix} = a\begin{pmatrix}1 & 1 \\ 1 & -1\end{pmatrix}\begin{pmatrix}|1\rangle \\ |2\rangle\end{pmatrix}$$

即可以将 $\hat{H}$ 用矩阵表示为：

$$\hat{H} = a\begin{pmatrix}1 & 1 \\ 1 & -1\end{pmatrix}$$

下面计算 $\hat{H}$ 的本征值和本征矢：

$$\begin{aligned}
\det(\hat{H} - E\hat{I}) &= \begin{vmatrix}a-E & a \\ a & -a-E\end{vmatrix} = 0 \\
&\Rightarrow (a-E)(-a-E) - a^2 = 0 \\
&\Rightarrow E = \pm\sqrt{2}a
\end{aligned}$$

1. $E_1 = \sqrt{2}a$ 时，有

$$\begin{aligned}
(\hat{H} - E_1\hat{I})|\psi_1\rangle &= \begin{pmatrix}a-\sqrt{2}a & a \\ a & -a-\sqrt{2}a\end{pmatrix}\begin{pmatrix}c_1 \\ c_2\end{pmatrix} = 0 \\
&\Rightarrow c_1 = (1+\sqrt{2})c_2 \\
&\Rightarrow |\psi_1\rangle = \frac{1}{\sqrt{(1)^2 + (1+\sqrt{2})^2}}((1+\sqrt{2})|1\rangle + |2\rangle) \\
&= \frac{1}{\sqrt{4+2\sqrt{2}}}((1+\sqrt{2})|1\rangle + |2\rangle)
\end{aligned}$$

2. $E_2 = -\sqrt{2}a$ 时，有

$$\begin{aligned}
(\hat{H} - E_2\hat{I})|\psi_2\rangle &= \begin{pmatrix}a+\sqrt{2}a & a \\ a & -a+\sqrt{2}a\end{pmatrix}\begin{pmatrix}c_1 \\ c_2\end{pmatrix} = 0 \\
&\Rightarrow c_1 = (1-\sqrt{2})c_2 \\
&\Rightarrow |\psi_2\rangle = \frac{1}{\sqrt{(1)^2 + (1-\sqrt{2})^2}}((1-\sqrt{2})|1\rangle + |2\rangle) \\
&= \frac{1}{\sqrt{4-2\sqrt{2}}}((1-\sqrt{2})|1\rangle + |2\rangle)
\end{aligned}$$

综上所述，$\hat{H}$ 有两个本征值，对应两个本征矢，分别为：

1. $E_1 = \sqrt{2}a$, $|\psi_1\rangle = \frac{1}{\sqrt{4+2\sqrt{2}}}((1+\sqrt{2})|1\rangle + |2\rangle)$
2. $E_2 = -\sqrt{2}a$, $|\psi_1\rangle = \frac{1}{\sqrt{4-2\sqrt{2}}}((1-\sqrt{2})|1\rangle + |2\rangle)$

Problem3

(a)

已知

$$
\begin{aligned}
|\psi\rangle &= 9i\,|\phi_1\rangle + 2\,|\phi_2\rangle \\
|\chi\rangle &= -\frac{i}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle
\end{aligned}
$$

则下面计算 $|\psi\rangle\langle\chi|\,,|\chi\rangle\langle\psi|$

$$
\begin{aligned}
|\psi\rangle\langle\chi| &= (9i\,|\phi_1\rangle + 2\,|\phi_2\rangle)(\frac{i}{\sqrt{2}}\,\langle\phi_1| + \frac{1}{\sqrt{2}}\,\langle\phi_2|) \\
&= -\frac{9}{\sqrt{2}}\,|\phi_1\rangle\langle\phi_1| + \frac{9i}{\sqrt{2}}\,|\phi_1\rangle\langle\phi_2| + \frac{2i}{\sqrt{2}}\,|\phi_2\rangle\langle\phi_1| + \sqrt{2}\,|\phi_2\rangle\langle\phi_2|
\end{aligned}
$$

$$
\begin{aligned}
|\chi\rangle\langle\psi| &= (-\frac{i}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle)(-9i\,\langle\phi_1| + 2\,\langle\phi_2|) \\
&= -\frac{9}{\sqrt{2}}\,|\phi_1\rangle\langle\phi_1| - \frac{2i}{\sqrt{2}}\,|\phi_1\rangle\langle\phi_2| - \frac{9i}{\sqrt{2}}\,|\phi_2\rangle\langle\phi_1| + \sqrt{2}\,|\phi_2\rangle\langle\phi_2|
\end{aligned}
$$

显然，$|\psi\rangle\langle\chi| \neq |\chi\rangle\langle\psi|$

(b)

下面计算 $\mathrm{Tr}(|\psi\rangle\langle\chi|), \mathrm{Tr}(|\chi\rangle\langle\psi|)$

$$
\begin{aligned}
\mathrm{Tr}(|\psi\rangle\langle\chi|) &= -\frac{9}{\sqrt{2}} + \sqrt{2} = -\frac{7}{\sqrt{2}} \\
\mathrm{Tr}(|\chi\rangle\langle\psi|) &= -\frac{9}{\sqrt{2}} + \sqrt{2} = -\frac{7}{\sqrt{2}}
\end{aligned}
$$

显然，$\mathrm{Tr}(|\psi\rangle\langle\chi|) = \mathrm{Tr}(|\chi\rangle\langle\psi|)$

(c)

下面计算 $|\psi\rangle\langle\psi|\,,|\chi\rangle\langle\chi|$

$$
\begin{aligned}
|\psi\rangle\langle\psi| &= (9i\,|\phi_1\rangle + 2\,|\phi_2\rangle)(-9i\,\langle\phi_1| + 2\,\langle\phi_2|) \\
&= 81\,|\phi_1\rangle\langle\phi_1| + 18i\,|\phi_1\rangle\langle\phi_2| - 18i\,|\phi_2\rangle\langle\phi_1| + 4\,|\phi_2\rangle\langle\phi_2| \\
&= \begin{pmatrix} 81 & 18i \\ -18i & 4 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
|\chi\rangle\langle\chi| &= (-\frac{i}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle)(\frac{i}{\sqrt{2}}\,\langle\phi_1| + \frac{1}{\sqrt{2}}\,\langle\phi_2|) \\
&= \frac{1}{2}\,|\phi_1\rangle\langle\phi_1| - \frac{i}{2}\,|\phi_1\rangle\langle\phi_2| + \frac{i}{2}\,|\phi_2\rangle\langle\phi_1| + \frac{1}{2}\,|\phi_2\rangle\langle\phi_2| \\
&= \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}
\end{aligned}
$$

下面计算 $\mathrm{Tr}(|\psi\rangle\langle\psi|),\mathrm{Tr}(|\chi\rangle\langle\chi|)$

$$\begin{aligned}
\mathrm{Tr}(|\psi\rangle\langle\psi|) &= 81+4=85 \\
\mathrm{Tr}(|\chi\rangle\langle\chi|) &= \frac{1}{2}+\frac{1}{2}=1
\end{aligned}$$

当算符满足 $\hat{P}^\dagger=\hat{P},\hat{P}^2=\hat{P}$ 时，这便是一个投影算符。

显然，$|\psi\rangle\langle\psi|$ 不满足第二条性质，所以不是投影算符；而 $|\chi\rangle\langle\chi|$ 两条性质都满足，所以是一个投影算符。

Problem4

(a)

已知 $\hat{H}=\alpha(|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|)$

当算符满足 $\hat{P}^\dagger=\hat{P},\hat{P}^2=\hat{P}$ 时，这便是一个投影算符。

首先检查 $\hat{P}^\dagger=\hat{P}$:

$$\begin{aligned}
\hat{H}^\dagger &= \alpha^\dagger(|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|)^\dagger \\
&= \alpha(|\phi_2\rangle\langle\phi_1|+|\phi_1\rangle\langle\phi_2|)\equiv\hat{H}
\end{aligned}$$

然后检查 $\hat{P}^2=\hat{P}$:

$$\begin{aligned}
\hat{H}^2 &= \alpha^2(|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|)^2 \\
&= \alpha^2\left[|\phi_1\rangle\langle\phi_2||\phi_1\rangle\langle\phi_2|+|\phi_1\rangle\langle\phi_2||\phi_2\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_1||\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1||\phi_2\rangle\langle\phi_1|\right]
\end{aligned}$$

注意到 $\langle\phi_2|\phi_1\rangle=0,\langle\phi_1|\phi_1\rangle=1,\langle\phi_2|\phi_2\rangle=1$ ，则上式可以化简为：

$$\hat{H}^2=\alpha^2(|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|)\neq\hat{H}$$

所以 $\hat{H}$ 不是投影算符。

而 $\alpha^{-2}\hat{H}^2=(|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|)$ ，有：

$$(\alpha^{-2}\hat{H}^2)^\dagger=(|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|)^\dagger=((|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|))\equiv\alpha^{-2}\hat{H}^2$$

$$\begin{aligned}
(|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|)^2 &= (|\phi_1\rangle\langle\phi_1|\cdot|\phi_1\rangle\langle\phi_1|+|\phi_1\rangle\langle\phi_1|\cdot|\phi_2\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_2|\cdot|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|\cdot|\phi_2\rangle\langle\phi_2|) \\
&= (|\phi_1\rangle\langle\phi_1|+|\phi_2\rangle\langle\phi_2|)
\end{aligned}$$

所以 $\alpha^{-2}\hat{H}^2$ 是投影算符。

(b)

下面计算 $\hat{H}|\phi_1\rangle,\hat{H}|\phi_2\rangle$:

$$\begin{aligned}
\hat{H}|\phi_1\rangle &= \alpha(|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|)\cdot|\phi_1\rangle \\
&= \alpha|\phi_2\rangle \\
\hat{H}|\phi_2\rangle &= \alpha(|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|)\cdot|\phi_2\rangle \\
&= \alpha|\phi_1\rangle
\end{aligned}$$

所以，$|\phi_1\rangle,|\phi_2\rangle$ 都不是 $\hat{H}$ 的本征矢。

(c)

下面计算对易子 $[\hat{H}, |\phi_1\rangle\langle\phi_1|], [\hat{H}, |\phi_2\rangle\langle\phi_2|]$:

$$\begin{aligned}
[\hat{H}, |\phi_1\rangle\langle\phi_1|] &= \hat{H}|\phi_1\rangle\langle\phi_1| - |\phi_1\rangle\langle\phi_1|\hat{H} \\
&= \alpha|\phi_2\rangle\langle\phi_1| - |\phi_1\rangle\langle\phi_1| \cdot \alpha(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|) \\
&= \alpha|\phi_2\rangle\langle\phi_1| - \alpha|\phi_1\rangle\langle\phi_2| - 0 \\
&= \alpha(|\phi_2\rangle\langle\phi_1| - |\phi_1\rangle\langle\phi_2|)
\end{aligned}$$

$$\begin{aligned}
[\hat{H}, |\phi_2\rangle\langle\phi_2|] &= \hat{H}|\phi_2\rangle\langle\phi_2| - |\phi_2\rangle\langle\phi_2|\hat{H} \\
&= \alpha|\phi_1\rangle\langle\phi_2| - |\phi_2\rangle\langle\phi_2| \cdot \alpha(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|) \\
&= \alpha|\phi_1\rangle\langle\phi_2| - 0 - \alpha|\phi_2\rangle\langle\phi_1| \\
&= \alpha(|\phi_1\rangle\langle\phi_2| - |\phi_2\rangle\langle\phi_1|)
\end{aligned}$$

显然，两者之间存在关系：

$$[\hat{H}, |\phi_1\rangle\langle\phi_1|] + [\hat{H}, |\phi_2\rangle\langle\phi_2|] \equiv 0$$

(d)

若 $|\psi\rangle$ 是 $\hat{H}$ 的本征矢，则有

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

假设 $|\psi\rangle$ 仅由 $\{|\phi_1\rangle, |\phi_2\rangle\}$ 线性组成，即 $|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$
则可有如下计算：

$$\begin{gathered}
\hat{H}|\psi\rangle = E|\psi\rangle \\
\hat{H}(c_1|\phi_1\rangle + c_2|\phi_2\rangle) = E(c_1|\phi_1\rangle + c_2|\phi_2\rangle) \\
\alpha(c_1|\phi_2\rangle + c_2|\phi_1\rangle) = E(c_1|\phi_1\rangle + c_2|\phi_2\rangle) \\
\Rightarrow (\alpha c_2 - Ec_1)|\phi_1\rangle + (\alpha c_1 - Ec_2)|\phi_2\rangle = 0 \\
\Rightarrow \begin{cases} \alpha c_2 - Ec_1 = 0 \\ \alpha c_1 - Ec_2 = 0 \end{cases}
\end{gathered}$$

其非平凡解为 $E = \pm\alpha$

1. 当 $E_1 = \alpha$ 时，有 $c_1 = c_2 \Rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle + |\phi_2\rangle)$
2. 当 $E_2 = -\alpha$ 时，有 $c_1 = -c_2 \Rightarrow |\psi_2\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle - |\phi_2\rangle)$

这两个本征矢满足：$\langle\psi_1|\psi_2\rangle = \frac{1}{2}(\langle\phi_1| + \langle\phi_2|) \cdot (|\phi_1\rangle - |\phi_2\rangle) = \frac{1}{2}(1 - 0 + 0 - 1) = 0$
即这两个本征矢正交。

(e)

若 $\{|\phi_1\rangle, |\phi_2\rangle\}$ 构成一组完备正交基，则 $\hat{H}$ 可用矩阵表示：

$$\begin{aligned}\hat{H} &= \alpha(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|) \\ &= \alpha\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{aligned}$$

下面计算 $\hat{H}$ 的本征值和本征矢：

$$\begin{aligned}\det(\hat{H} - E\hat{I}) = \begin{vmatrix}-E & \alpha\\ \alpha & -E\end{vmatrix} = 0 \\ \Rightarrow E = \pm\alpha\end{aligned}$$

1. 当 $E_1 = \alpha$ 时，有：

$$\begin{aligned}(\hat{H} - E_1\hat{I})|\psi_1\rangle = \begin{pmatrix}-\alpha & \alpha\\ \alpha & -\alpha\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} = 0 \\ \Rightarrow c_1 = c_2 \\ \Rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle + |\phi_2\rangle)\end{aligned}$$

2. 当 $E_2 = -\alpha$ 时，有：

$$\begin{aligned}(\hat{H} - E_2\hat{I})|\psi_2\rangle = \begin{pmatrix}\alpha & \alpha\\ \alpha & \alpha\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} = 0 \\ \Rightarrow c_1 = -c_2 \\ \Rightarrow |\psi_2\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle - |\phi_2\rangle)\end{aligned}$$

综上所述，可以找到 $\hat{H}$ 的两个正交的本征矢，对应两个本征值，分别为：

1. $E_1 = \alpha$,$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle + |\phi_2\rangle)$
2. $E_2 = -\alpha$,$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle - |\phi_2\rangle)$

这两个本征矢与 (d) 中的一致。

Problem5

由图可知：

$$\begin{aligned}\hat{n} &= (\sin\beta\cos\alpha, \sin\beta\sin\alpha, \cos\beta) \\ \Rightarrow \hat{S}\cdot\hat{n} &= S_x\sin\beta\cos\alpha + S_y\sin\beta\sin\alpha + S_z\cos\beta \\ &= \frac{\hbar}{2}\left\{(|+\rangle\langle-| + |-\rangle\langle+|)\sin\beta\cos\alpha + i(-|+\rangle\langle-| + |-\rangle\langle+|)\sin\beta\sin\alpha + (|+\rangle\langle+| - |-\rangle\langle-|)\cos\beta\right\} \\ &= \frac{\hbar}{2}\left\{(\sin\beta\cos\alpha - i\sin\beta\sin\alpha)|+\rangle\langle-| + (\sin\beta\cos\alpha + i\sin\beta\sin\alpha)|-\rangle\langle+| + \cos\beta|+\rangle\langle+| - \cos\beta|-\rangle\langle-|\right\} \\ &= \frac{\hbar}{2}\left\{\sin\beta e^{-i\alpha}|+\rangle\langle-| + \sin\beta e^{i\alpha}|-\rangle\langle+| + \cos\beta|+\rangle\langle+| - \cos\beta|-\rangle\langle-|\right\}\end{aligned}$$

假设 $|\hat{S}\cdot\hat{n};+\rangle = c_+|+\rangle + c_-|-\rangle$ ，有以下计算：

$$\hat{S}\cdot\hat{n}|\hat{S}\cdot\hat{n};+\rangle = (\frac{\hbar}{2})|\hat{S}\cdot\hat{n};+\rangle$$

$$\begin{aligned}
\text{左边} &= \frac{\hbar}{2}\{\sin\beta e^{-i\alpha}|+\rangle\langle-| + \sin\beta e^{i\alpha}|-\rangle\langle+| + \cos\beta|+\rangle\langle+| - \cos\beta|-\rangle\langle-|\}\cdot|\hat{S}\cdot\hat{n};+\rangle \\
&= \frac{\hbar}{2}\{\sin\beta e^{-i\alpha}|+\rangle\langle-| + \sin\beta e^{i\alpha}|-\rangle\langle+| + \cos\beta|+\rangle\langle+| - \cos\beta|-\rangle\langle-|\}\cdot(c_+|+\rangle + c_-|-\rangle) \\
&= \frac{\hbar}{2}(\sin\beta e^{i\alpha}c_+|-\rangle + \cos\beta c_+|+\rangle + \sin\beta e^{-i\alpha}c_-|+\rangle - \cos\beta c_-|-\rangle) \\
&= \frac{\hbar}{2}\{(\sin\beta e^{-i\alpha}c_- + \cos\beta c_+)|+\rangle + (\sin\beta e^{i\alpha}c_+ - \cos\beta c_-)|-\rangle\} = (\frac{\hbar}{2})(c_+|+\rangle + c_-|-\rangle) \\
&\Rightarrow \begin{cases} \sin\beta e^{-i\alpha}c_- + \cos\beta c_+ = c_+ \\ \sin\beta e^{i\alpha}c_+ - \cos\beta c_- = c_- \end{cases} \\
&\Rightarrow \cos\frac{\beta}{2}c_- = e^{i\alpha}\sin\frac{\beta}{2}c_+ \\
&\Rightarrow |\hat{S}\cdot\hat{n};+\rangle = \cos\frac{\beta}{2}|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}|-\rangle
\end{aligned}$$

下面验证 $|\hat{S}\cdot\hat{n};+\rangle$ 已经正交归一：

$$\begin{aligned}
\langle\hat{S}\cdot\hat{n};+|\hat{S}\cdot\hat{n};+\rangle &= (\cos\frac{\beta}{2}\langle+| + e^{-i\alpha}\sin\frac{\beta}{2}\langle-|)(\cos\frac{\beta}{2}|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}|-\rangle) \\
&= (\cos\frac{\beta}{2})^2 + (\sin\frac{\beta}{2})^2 = 1
\end{aligned}$$

综上所述，$|\hat{S}\cdot\hat{n};+\rangle = \cos\frac{\beta}{2}|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}|-\rangle$ 即是满足要求的态。