Quantum Mechanics
1. Quantum State and Hilbert Space
Solving Problems

Problem 1

If the states $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis and if the operator $\hat{K}$ has the properties

$$\hat{K}|1\rangle = 2|1\rangle$$
$$\hat{K}|2\rangle = 3|2\rangle$$
$$\hat{K}|3\rangle = -6|3\rangle$$

(a) Write an expression for $\hat{K}$ in terms of its eigenvalues and eigenvectors (projection operators). Use this expression to derive the matrix representing $\hat{K}$ in the $|1\rangle, |2\rangle, |3\rangle$ basis.

(b) What is the expectation or average value of $\hat{K}$, defined as $\langle\alpha|\hat{K}|\alpha\rangle$, in the state

$$|\alpha\rangle = \frac{1}{4}(-3|1\rangle + i\sqrt{6}|2\rangle + |3\rangle)$$

1.1 a

对于题目中给定的算符的性质可知：由于 $\{|1\rangle, |2\rangle, |3\rangle\}$ 是一组正交归一基，即 $\langle 1|1\rangle = 1$，即可得如下形式：

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

根据此形式即可得出 $\hat{K}$ 在 $|1\rangle, |2\rangle, |3\rangle$ 基中的矩阵表示：

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

1.2 b

对于 $|\alpha\rangle = \dfrac{1}{4}(-3|1\rangle + i\sqrt{6}|2\rangle + |3\rangle)$
可知其左矢为：$\frac{1}{4}((-3)^\dagger\langle 1| + (i\sqrt{6})^\dagger\langle 2| + \langle 3|)$
根据 $\{|1\rangle, |2\rangle, |3\rangle\}$ 为一组正交归一基，所以 $\langle m|n\rangle = 0$

所以可得

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

Problem 2

The Hamiltonian operator for a two-state system is given by

$$H = a(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|),$$

where a is a number with the dimension of energy. Find the energy eigenvalues and the corresponding energy eigenkets (as linear combinations of $|1\rangle$ and $|2\rangle$).

解：对于问题中所给出的哈密顿算符有：

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

所以此哈密顿算符可以表示为：

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

根据线性代数可知，其本征值满足：

$$\det\left(\hat{H} - \lambda I\right) = 0,$$

即：

$$\det\begin{pmatrix}a-\lambda & a\\a & -a-\lambda\end{pmatrix} = 0.$$

$$(a-\lambda)(-a-\lambda) - a^2 = 0,$$

因此本征值为：

$$\lambda_1 = \sqrt{2}a,\quad \lambda_2 = -\sqrt{2}a.$$

对于 $\lambda_1 = \sqrt{2}a$

$$(\hat{H} - \lambda I)|v_1\rangle = \begin{pmatrix}a-\sqrt{2}a & a\\a & -a-\sqrt{2}a\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = 0$$

解得：

$$c_1 = (1+\sqrt{2})c_2$$

即：

$$|v_1\rangle == \frac{1}{\sqrt{4+2\sqrt{2}}}((1+\sqrt{2})|1\rangle + |2\rangle)$$

同理可得：在 $\lambda_2 = -\sqrt{2}a$ 时，本征矢为：

$$|v_2\rangle = \frac{1}{\sqrt{4-2\sqrt{2}}}((1-\sqrt{2})|1\rangle + |2\rangle)$$

Problem 3

Consider the states $|\psi\rangle = 9i\,|\phi_1\rangle + 2\,|\phi_2\rangle$ and $|\chi\rangle = -\frac{i}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle$ where the two vectors $|\phi_1\rangle$and $|\phi_2\rangle$ form a complete and orthonormal basis.

(a) Calculate the operators $|\psi\rangle\langle\chi|$ and $|\chi\rangle\langle\psi|$. Are they equal? item Find the Hermitian conjugates of $|\psi\rangle, |\chi\rangle, |\psi\rangle\langle\chi|$, and $|\chi\rangle\langle\psi|$.

(b) Calculate $\mathrm{Tr}(|\psi\rangle\langle\chi|)$ and $\mathrm{Tr}(|\chi\rangle\langle\psi|)$. Are they equal?

(c) Calculate $|\psi\rangle\langle\psi|$ and $\chi\rangle\langle\chi|$ and the traces $\mathrm{Tr}(|\psi\rangle\langle\psi|)$ and $\mathrm{Tr}(|\chi\rangle\langle\chi|)$. Are they projection operators?

3.1 a

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

二者并不相等。

3.2 b

$$\mathrm{TR}(|\psi\rangle\langle\chi|) = -\frac{9}{\sqrt{2}} + \sqrt{2} = -\frac{7}{\sqrt{2}} \quad \mathrm{TR}(|\chi\rangle\langle\psi|) = -\frac{9}{\sqrt{2}} + \sqrt{2} = -\frac{7}{\sqrt{2}}$$

二者相等。

3.3 c

$$
\begin{aligned}
|\psi\rangle\langle\psi| &= (9i\,|\phi_1\rangle + 2\,|\phi_2\rangle)(-9i\,\langle\phi_1| + 2\,\langle\phi_2|) \\
&= 81\,|\phi_1\rangle\,\langle\phi_1| + 18i\,|\phi_1\rangle\,\langle\phi_2| - 18i\,|\phi_2\rangle\,\langle\phi_1| + 4\,|\phi_2\rangle\,\langle\phi_2| \\
&= \begin{pmatrix} 81 & 18i \\ -18i & 4 \end{pmatrix} \\
|\chi\rangle\langle\chi| &= (-\frac{i}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle)(\frac{i}{\sqrt{2}}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2|) \\
&= \frac{1}{2}|\phi_1\rangle\langle\phi_1| - \frac{i}{2}|\phi_1\rangle\langle\phi_2| + \frac{i}{2}|\phi_2\rangle\langle\phi_1| + \frac{1}{2}|\phi_2\rangle\langle\phi_2 \\
&= \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}
\end{aligned}
$$

对于投影算符来说，其为厄米算符且具备幂等性。

对于二者来说：$|\psi\rangle\langle\psi|$ 不满足第二条性质, 所以不是投影算符。而 $|\chi\rangle\langle\chi|$ 是一个投影算符。

Problem 4