Problem 1 – Chapter 6 # 1)
Let $|\phi_n\rangle$ be the eigenstates of a Hamiltonian $\hat{H}$ (a hermitian operator). Assume that the $|\phi_n\rangle$ form a discrete orthonormal basis. Consider the operator $\hat{U}(m,n)$ defined as

$$\hat{U}(m,n) = |\phi_m\rangle \langle\phi_n| . \tag{1}$$

(a) Obtain the adjoint $\hat{U}^\dagger(m,n)$.
(b) Evaluate the commutator $[\hat{H}, \hat{U}(m,n)]$.
(c) Show that

$$\hat{U}(m,n)\hat{U}^\dagger(p,q) = \delta_{nq}\hat{U}(m,p). \tag{2}$$

(d) Calculate the trace of $\hat{U}(m,n)$. The trace of an operator $\hat{A}$ is defined as

$$\mathrm{Tr}\Big(\hat{A}\Big) = \sum_n \langle\phi_n| \hat{A} |\phi_n\rangle . \tag{3}$$

(e) If $\hat{A}$ is an operator with matrix elements $A_{mn} = \langle\phi_m| \hat{A} |\phi_n\rangle$, show that

$$\hat{A} = \sum_{m,n} A_{mn}\hat{U}(m,n). \tag{4}$$

(f) Show that

$$A_{pq} = \mathrm{Tr}\Big[\hat{A}\hat{U}^\dagger(p,q)\Big]. \tag{5}$$

(a) The adjoint $A^\dagger$ is defined such that $\langle\psi| A^\dagger$ is dual to $A|\psi\rangle$. Notice that $\hat{U}(m,n)|\psi\rangle = |\phi_m\rangle\langle\phi_n|\psi\rangle$ whose dual is $\langle\psi|\hat{U}^\dagger = \langle\phi_n|\psi\rangle^* \langle\phi_m| = \langle\psi|\phi_n\rangle\langle\phi_m|$. Thus, $\hat{U}^\dagger(m,n) = |\phi_n\rangle\langle\phi_m| = \hat{U}(n,m)$.

(b) The commutator

$$\begin{aligned}[\hat{H}, \hat{U}(m,n)] &= \hat{H}|\phi_m\rangle\langle\phi_n| - |\phi_m\rangle\langle\phi_n|\hat{H} = E_m|\phi_m\rangle\langle\phi_n| - |\phi_m\rangle\langle\phi_n| E_n \\ &= (E_m - E_n)\hat{U}(m,n).\end{aligned} \tag{6}$$

(c) Using the fact that $\{|\phi_n\rangle\}$ is orthonormal

$$\hat{U}(m,n)\hat{U}^\dagger(p,q) = |\phi_m\rangle\langle\phi_n|\phi_q\rangle\langle\phi_p| = \delta_{nq}|\phi_m\rangle\langle\phi_p| = \delta_{nq}\hat{U}(m,p). \tag{7}$$

(d) The trace of $\hat{U}(m,n)$ is

$$\mathrm{Tr}\Big(\hat{U}(m,n)\Big) = \sum_k \langle\phi_k|\phi_m\rangle\langle\phi_n|\phi_k\rangle = \sum_k \delta_{km}\delta_{nk} = \delta_{nm}. \tag{8}$$

(e) Since $\{|\phi_n\rangle\}$ forms an orthonormal basis

$$\hat{A} = \hat{\mathbb{1}}\hat{A}\hat{\mathbb{1}} = \sum_{n,m} |\phi_m\rangle \underbrace{\langle\phi_m|\,\hat{A}\,|\phi_n\rangle}_{A_{mn}} \langle\phi_n| = \sum_{n,m} A_{mn}\hat{U}(m,n). \tag{9}$$

(f) Using the results above, we find

$$\hat{A}\hat{U}^\dagger(p,q) = \sum_{m,n} A_{mn}\hat{U}(m,n)\hat{U}^\dagger(p,q) = \sum_{m} A_{mq}\hat{U}(m,p) \tag{10}$$

and

$$\mathrm{Tr}\Big(\hat{A}\hat{U}^\dagger(p,q)\Big) = \sum_{m} A_{mq}\delta_{mp} = A_{pq}. \tag{11}$$

Problem 2 – Chapter 7 # 4)
Consider the Hamiltonian $\hat{H}$ of a particle in a one-dimensional problem given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x}), \tag{12}$$

where $\hat{x}$ and $\hat{p}$ are the position and momentum operators satisfying the standard commutation relations. Let $|\phi_n\rangle$ be the eigenstates of $\hat{H}$ with $\hat{H}\,|\phi_n\rangle = E_n\,|\phi_n\rangle$, where n is a discrete index.
(a) By considering the commutator $[\hat{x}, \hat{H}]$, show that

$$\langle\phi_m|\,\hat{p}\,|\phi_n\rangle = \alpha_{mn}\,\langle\phi_m|\,\hat{x}\,|\phi_n\rangle\,, \tag{13}$$

where the coefficient α_{mn} depends on the energy difference $E_m - E_n$.
(b) Using the closure relation satisfied by the eigenstates of $\hat{H}$ and the result above, deduce the following relation (sum rule)

$$\sum_n (E_m - E_n)^2 |\,\langle\phi_m|\,\hat{x}\,|\phi_n\rangle\,|^2 = \frac{\hbar^2}{m^2}\,\langle\phi_m|\,\hat{p}^2\,|\phi_n\rangle\,. \tag{14}$$

(a) Consider the generic operators $\hat{A}, \hat{B}, \hat{C}$. The commutator

$$\begin{aligned}
[\hat{A}, \hat{B}\hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}].
\end{aligned} \tag{15}$$

We can use this and the assumption that $[\hat{x}, \hat{p}] = i\hbar$ to find

$$[\hat{x}, \hat{p}^2] = [\hat{x}, \hat{p}]\hat{p} + \hat{p}[\hat{x}, \hat{p}] = 2i\hbar\hat{p}, \tag{16}$$

and therefore,

$$[\hat{x}, \hat{H}] = \frac{1}{2m}[\hat{x}, \hat{p}^2] + [\hat{x}, \hat{V}(\hat{x})] = \frac{i\hbar}{m}\hat{p}. \tag{17}$$

Thus, the matrix elements of the commutator

$$\langle\phi_m| [\hat{x}, \hat{H}] |\phi_n\rangle = (E_n - E_m) \langle\phi_m| \hat{x} |\phi_n\rangle = \frac{i\hbar}{m} \langle\phi_m| \hat{p} |\phi_n\rangle . \tag{18}$$

Rearranging, we find

$$\langle\phi_m| \hat{p} |\phi_n\rangle = \underbrace{\frac{im}{\hbar}(E_m - E_n)}_{\alpha_{mn}} \langle\phi_m| \hat{x} |\phi_n\rangle . \tag{19}$$

(b) Observe the following:

$$(E_m - E_n)^2 | \langle\phi_m| \hat{x} |\phi_n\rangle |^2 = \frac{\hbar^2}{m} | \langle\phi_m| \hat{p} |\phi_n\rangle |^2. \tag{20}$$

Problem 3 – Chapter 6 # 13)
Consider a three-dimensional state space. If a certain set of orthonormal kets $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ are used as the base kets, the operators $\hat{A}$ and $\hat{B}$ are represented by

$$A = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \quad B = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}, \tag{21}$$

where a and b are real.
(a) It is obvious that $\hat{A}$ has a degenerate spectrum. Is the spectrum of $\hat{B}$ also degenerate?
(b) Show that $\hat{A}$ and $\hat{B}$ commute.
(c) Find a new set of orthonormal kets which are simultaneous eigenstates of both $\hat{A}$ and $\hat{B}$. Specify the eigevalues of $\hat{A}$ and $\hat{B}$ for each of these three eigenstates. Does specifying these eigenvalues uniquely identify the relative common eigenstate? That is, do $\hat{A}$ and $\hat{B}$ form a complete set of commuting observables?

(a) Let $|\phi_1\rangle$ correspond to eigenvalue a of $\hat{A}$ and $|\phi_2\rangle, |\phi_3\rangle$ correspond to $-a$. Thus, $|\phi_1\rangle$ also corresopnds to eigenvalue b of $\hat{B}$. The other eigenvalues of $\hat{B}$ will have eigenvectors which are linear combinations of $|\phi_2\rangle, |\phi_3\rangle$, meaning that we only have to diagonalize

$$\begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix}. \tag{22}$$

It should be clear that this matrix has characteristic equation $\lambda^2 - b^2 = 0$, which has roots $\lambda = \pm b$. Thus, $\hat{B}$ also has a degenerate spectrum.

(b) Taking the matrix products explicitly, we find

$$AB - BA = \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} - \begin{pmatrix} ba & 0 & 0 \\ 0 & 0 & iba \\ 0 & -iba & 0 \end{pmatrix} = 0. \tag{23}$$

Since the mapping between the matrix representation and hilbert space are bijective, the commutation holds for the operators $\hat{A}$ and $\hat{B}$ in the hilbert space.

(c) In part (a), we found the spectrum of $\hat{B}$. Now, we solve for the eigenvectors in the supspace spanned by $|\phi_2\rangle$ and $|\phi_3\rangle$, which have the general form $\begin{pmatrix}\alpha_1 & \alpha_2\end{pmatrix}^T$:

$$-ib\alpha_2 = \pm b\alpha_1 \Rightarrow \alpha_2 = \pm i\alpha_1. \tag{24}$$

The eigenvector corresponding to eigenvalue $\pm b$ is then

$$\frac{1}{\sqrt{2}}\Big[\,|\phi_2\rangle \pm i\,|\phi_3\rangle\,\Big]. \tag{25}$$

It should be clear that these eigenvectors of $\hat{B}$ are still eigenvectors of $\hat{A}$ corresponding to eigenvalue $-a$. Furthermore, the correspondence between eigenvalues and eigenvectors is given by

$$\{a, b\} \leftrightarrow |\phi_1\rangle \tag{26}$$

$$\{-a, b\} \leftrightarrow (|\phi_2\rangle + i\,|\phi_3\rangle)/\sqrt{2} \tag{27}$$

$$\{-a, -b\} \leftrightarrow (|\phi_2\rangle - i\,|\phi_3\rangle)/\sqrt{2}. \tag{28}$$

It is obvious then that specifying the eigenvalues of $\hat{A}$ and $\hat{B}$ uniquely specifies the simultaneous corresponding eigenvector of $\hat{A}$ and $\hat{B}$, meaning that $\hat{A}$ and $\hat{B}$ form a complete set of commuting observables.

Problem 4 – Chapter 6 # 14)

A molecule is composed of six identical atoms $A_1, A_2, \ldots, A_6$ which form a regular hexagon. Consider an electron which can be localized on each of the atoms. Denote with $|\psi_n\rangle$ the state in which the electron is localized on the n^{th} atom ($n = 1, 2, \ldots, 6$). The electron states will be limited to the space spanned by the $|\psi_n\rangle$, assumed to be orthonormal $\langle\psi_m|\psi_n\rangle = \delta_{mn}$; in other words, these six states form a basis.

(a) Define the operator $\hat{R}$ by the following relations:

$$\hat{R}\,|\psi_1\rangle = |\psi_2\rangle\,, \quad \hat{R}\,|\psi_2\rangle = |\psi_3\rangle\,, \quad \ldots, \quad \hat{R}\,|\psi_6\rangle = |\psi_1\rangle\,. \tag{29}$$

Find the eigenvalues and eigenstates of $\hat{R}$. Show that the eigenvectors form an orthonormal set (i.e. they form a basis).

(b) Show that the adjoint operator $\hat{R}^\dagger$ gives

$$\hat{R}^\dagger\,|\psi_1\rangle = |\psi_6\rangle\,, \quad \hat{R}^\dagger\,|\psi_2\rangle = |\psi_1\rangle\,, \quad \ldots, \quad \hat{R}^\dagger\,|\psi_6\rangle = |\psi_5\rangle\,. \tag{30}$$

Show that $\hat{R}$ is unitary.
(c) When the probability of the electron jumping from one site to a contiguous one to the left or right is neglected, its energy is described by the Hamiltonian $\hat{H}_0$, whose eigenstates are the six states $|\psi_n\rangle$, all with the same eigenvalue E_0, namely $\hat{H}_0 |\psi_n\rangle = E_0 |\psi_n\rangle$. The possibility for the electron to jump from one site to another is modeled by adding the Hamiltonian $\hat{H}_0$ a perturbation $\hat{V}$ such that

$$\begin{aligned} &\hat{V} |\psi_1\rangle = -a |\psi_6\rangle - a |\psi_2\rangle, \quad \hat{V} |\psi_2\rangle = -a |\psi_1\rangle - a |\psi_3\rangle, \quad \dots, \\ &\hat{V} |\psi_6\rangle = -a |\psi_5\rangle - a |\psi_1\rangle. \end{aligned} \tag{31}$$

Show that $\hat{R}$ commutes with the total Hamiltonian $\hat{H} = \hat{H} + \hat{V}$. From this deduce the eigenstates and eigenvalues of $\hat{H}$. In these eigenstates is the electron localized?
Hint: The N distinct complex roots of $z^N = 1$ are given by $z_n = e^{i(2\pi n/N)}$ for $n = 1, 2, \dots, N$, and the following identity holds:

$$\sum_{n=0}^{N} z^n = \frac{1 - z^{N+1}}{1 - z} \tag{32}$$

for complex z.

(a) The eigen-equation for $\hat{R}$ is $\hat{R} |\psi\rangle = r |\psi\rangle$. It is clear from the definition of $\hat{R}$ that $\hat{R}^6 = \hat{\mathbb{1}}$, meaning that

$$\hat{R}^6 |\psi\rangle = \hat{\mathbb{1}} |\psi\rangle = r^6 |\psi\rangle \Rightarrow r^6 = 1. \tag{33}$$

The eigenvalues of $\hat{R}$ are then just the sixth roots of unity: $\{e^{i\pi/3}, e^{i2\pi/3}, e^{i\pi}, e^{i4\pi/3}, e^{i5\pi/3}, 1\}$.