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)

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

(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:

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

If we sum over n on both sides we have

$$\sum_n (E_m - E_n)^2 |\langle\phi_m| \hat{x} |\phi_n\rangle|^2 = \frac{\hbar^2}{m^2} \langle\phi_m| \hat{p}^2 |\phi_m\rangle , \tag{21}$$

where we have used the fact that the states $\{|\phi_n\rangle\}$ are complete on the right. Note that this is not possible on the l.h.s. since the factor of the energy difference depends on n.

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

$$A = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \quad B = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}, \tag{22}$$

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

$$\begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix}. \tag{23}$$

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

$$AB - BA = \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} - \begin{pmatrix} ba & 0 & 0 \\ 0 & 0 & iba \\ 0 & -iba & 0 \end{pmatrix} = 0. \tag{24}$$

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 $\begin{pmatrix}\alpha_1 & \alpha_2\end{pmatrix}^T$:

$$-ib\alpha_2 = \pm b\alpha_1 \Rightarrow \alpha_2 = \pm i\alpha_1. \tag{25}$$

The eigenvectors corresponding to eigenvalues $\pm b$ is then

$$\frac{1}{\sqrt{2}}\Big[\, |\phi_2\rangle \pm i\,|\phi_3\rangle \,\Big]. \tag{26}$$

It should be clear that these eigenvectors of $\hat{B}$ are still eigenvectors of $\hat{A}$ corresponding to eigenvalue $-a$ and also that they are orthogonal to each other and $|\phi_1\rangle$. Furthermore, the correspondence between eigenvalues and eigenvectors is given by

$$\{a, b\} \leftrightarrow |\phi_1\rangle \tag{27}$$
$$\{-a, b\} \leftrightarrow (|\phi_2\rangle + i\,|\phi_3\rangle)/\sqrt{2} \tag{28}$$
$$\{-a, -b\} \leftrightarrow (|\phi_2\rangle - i\,|\phi_3\rangle)/\sqrt{2}. \tag{29}$$

It is clear 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:

$$\hat{R}\,|\psi_1\rangle = |\psi_2\rangle\,, \quad \hat{R}\,|\psi_2\rangle = |\psi_3\rangle\,, \quad \ldots, \quad \hat{R}\,|\psi_6\rangle = |\psi_1\rangle\,. \tag{30}$$

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

$$\hat{R}^\dagger\,|\psi_1\rangle = |\psi_6\rangle\,, \quad \hat{R}^\dagger\,|\psi_2\rangle = |\psi_1\rangle\,, \quad \ldots, \quad \hat{R}^\dagger\,|\psi_6\rangle = |\psi_5\rangle\,. \tag{31}$$

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

$$\begin{aligned} &\hat{V}\,|\psi_1\rangle = -a\,|\psi_6\rangle - a\,|\psi_2\rangle\,, \quad \hat{V}\,|\psi_2\rangle = -a\,|\psi_1\rangle - a\,|\psi_3\rangle\,, \quad \ldots, \\ &\hat{V}\,|\psi_6\rangle = -a\,|\psi_5\rangle - a\,|\psi_1\rangle\,. \end{aligned} \tag{32}$$

Show that $\hat{R}$ commutes with the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. 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 $n = 1, 2, \ldots, N$, and the following identity holds:

$$\sum_{n=0}^{N} z^n = \frac{1 - z^{N+1}}{1 - z} \tag{33}$$

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

$$\hat{R}^6\,|\psi\rangle = \hat{\mathbb{1}}\,|\psi\rangle = r^6\,|\psi\rangle \Rightarrow r^6 = 1. \tag{34}$$

The eigenvalues of $\hat{R}$ are then just the sixth roots of unity: $\{e^{i\pi/3}, e^{i2\pi/3}, e^{i\pi}, e^{i4\pi/3}, e^{i5\pi/3}, 1\}$. If we denote the n^{th} sixth root of unity as ω_n for $n = 1, \ldots, 6$, the eigenvectors can be found from

$$\begin{pmatrix} -\omega_n & 1 & 0 & 0 & 0 & 0 \\ 0 & -\omega_n & 1 & 0 & 0 & 0 \\ 0 & 0 & -\omega_n & 1 & 0 & 0 \\ 0 & 0 & 0 & -\omega_n & 1 & 0 \\ 0 & 0 & 0 & 0 & -\omega_n & 1 \\ 1 & 0 & 0 & 0 & 0 & -\omega_n \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} = 0. \tag{35}$$

Equivalently, we have the system of equations

$$\begin{cases} -\omega_n a_1 + a_2 = 0 \\ -\omega_n a_2 + a_3 = 0 \\ -\omega_n a_3 + a_4 = 0 \\ -\omega_n a_4 + a_5 = 0 \\ -\omega_n a_5 + a_6 = 0 \\ \quad a_1 - \omega_n a_6 = 0. \end{cases} \tag{36}$$

While it may not be clear from the system above, we know that these equations are linearly dependent with one free undetermined parameter since each eigenvalue has algebraic multiplicity 1. Thus, we can let a_1 be our undetermined parameter and solve for $a_2, \ldots, a_6$ in terms of a_1. Denoting the eigenvector corresponding to eigenvalue ω_n as $|\chi_n\rangle$, we find

$$\chi_n = a_1 \begin{pmatrix} 1 \\ \omega_n \\ \omega_n^2 \\ \omega_n^3 \\ \omega_n^4 \\ \omega_n^5 \end{pmatrix}. \tag{37}$$

This is a very nice form for the eigenvectors. Normalizing we find

$$\chi_n^\dagger \chi_n = 6|a_1|^2 = 1 \Rightarrow a_1 = 1/\sqrt{6}. \tag{38}$$

(b) In the basis $|\psi_1\rangle, \ldots, |\psi_6\rangle$

$$\hat{R} = |\psi_1\rangle\langle\psi_2| + |\psi_2\rangle\langle\psi_3| + |\psi_3\rangle\langle\psi_4| + |\psi_4\rangle\langle\psi_5| + |\psi_5\rangle\langle\psi_6| + |\psi_6\rangle\langle\psi_1|. \tag{39}$$

It is clear then that

$$\hat{R}^\dagger = |\psi_2\rangle\langle\psi_1| + |\psi_3\rangle\langle\psi_2| + |\psi_4\rangle\langle\psi_3| + |\psi_5\rangle\langle\psi_4| + |\psi_6\rangle\langle\psi_5| + |\psi_1\rangle\langle\psi_6|. \tag{40}$$

Thus, we have the actions

$$\hat{R}^\dagger |\psi_1\rangle = |\psi_6\rangle, \quad \hat{R}^\dagger |\psi_2\rangle = |\psi_1\rangle, \quad \ldots, \quad \hat{R}^\dagger |\psi_6\rangle = |\psi_5\rangle. \tag{41}$$

Furthermore, we have

$$R^\dagger R = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{42}$$

Hence, $\hat{R}$ is unitary (in the matrix representation R is orthogonal since it is real).

(c) It is clear that $[\hat{R}, \hat{H}_0] = 0$ since in the eigenbasis of $\hat{H}_0$, $\hat{H}_0 = E_0\hat{\mathbb{1}}$. Note that $\hat{V} = -a(\hat{R}^\dagger + \hat{R})$. From this, it is clear that $[\hat{R}, V] = 0$ since $\hat{R}$ commutes with itself and its adjoint[1]. It is clear that $\{|\chi_n\rangle\}$ forms a simultaneous orthonormal basis for $\hat{H}_0$ and $\hat{R}$. From the fact that $\hat{V} = -a(\hat{R}^\dagger + \hat{R})$ and that $\hat{R}^\dagger |\chi_n\rangle = \omega_n^* |\chi_n\rangle$, we have $\hat{V} |\chi_n\rangle = -(a/2)\,\mathrm{Re}(\omega_n)$. The eigenvalues of $\hat{H}$ are then given by $E_0 - (a/2)\cos(\pi n/3)$.

[1] This is not generally true – it is only the case here since $\hat{R}$ is unitary.