Quantum Mechanics

Solutions to the Problems in Homework Assignment 05

Fall, 2019

1. **[C-T Exercise 2-1]** $|\varphi_n\rangle$ are the eigenstates of a Hermitian operator $\hat{H}$ ($\hat{H}$ is, for example, the Hamiltonian of an arbitrary physical system). Assume that the states $|\varphi_n\rangle$ form a discrete orthonormal basis. The operator $\hat{U}(m,n)$ is defined by $\hat{U}(m,n) = |\varphi_m\rangle\langle\varphi_n|$.

   (a) Calculate the adjoint $\hat{U}^\dagger(m,n)$ of $\hat{U}(m,n)$.

   (b) Calculate the commutator $[\hat{H}, \hat{U}(m,n)]$.

   (c) Prove the relation $\hat{U}(m,n)\hat{U}^\dagger(p,q) = \delta_{nq}\hat{U}(m,p)$.

   (d) Calculate $\mathrm{Tr}\{\hat{U}(m,n)\}$, the trace of the operator $\hat{U}(m,n)$.

   (e) Let $\hat{A}$ be an operator, with matrix elements $A_{mn} = \langle\varphi_m|\hat{A}|\varphi_n\rangle$. Prove the relation $\hat{A} = \sum_{m,n} A_{mn}\hat{U}(m,n)$.

   (f) Show that $A_{pq} = \mathrm{Tr}\{\hat{A}U^\dagger(p,q)\}$.

(a) The adjoint $\hat{U}^\dagger(m,n)$ of $\hat{U}(m,n)$ is given by

$$\hat{U}^\dagger(m,n) = \big(|\varphi_m\rangle\langle\varphi_n|\big)^\dagger = |\varphi_n\rangle\langle\varphi_m|\,.$$

(b) The eigenequation of $\hat{H}$ reads

$$\hat{H}\,|\varphi_n\rangle = E_n\,|\varphi_n\rangle\,.$$

The orthonormality relation of the eigenvectors is given by

$$\langle\varphi_m|\varphi_n\rangle = \delta_{mn}.$$

The closure relation of the eigenvectors is given by

$$\hat{P}_{\{\varphi_n\}} = \sum_n |\varphi_n\rangle\langle\varphi_n| = 1.$$

Let $|\psi\rangle$ be an arbitrary ket in the state space of the physical system. Acting the commutator $[\hat{H}, \hat{U}(m,n)]$ on $|\psi\rangle$, we have

$$\begin{aligned}
[\hat{H}, \hat{U}(m,n)]\,|\psi\rangle &= \hat{H}\hat{U}(m,n)\,|\psi\rangle - \hat{U}(m,n)\hat{H}\,|\psi\rangle \\
&= \hat{H}\,|\varphi_m\rangle\langle\varphi_n|\psi\rangle - |\varphi_m\rangle\langle\varphi_n|\hat{H}|\psi\rangle \\
&= E_m\,|\varphi_m\rangle\langle\varphi_n|\psi\rangle - E_n\,|\varphi_m\rangle\langle\varphi_n|\psi\rangle \\
&= \big(E_m - E_n\big)\,|\varphi_m\rangle\langle\varphi_n|\psi\rangle \\
&= \big(E_m - E_n\big)\hat{U}(m,n)\,|\psi\rangle\,.
\end{aligned}$$

Because $|\psi\rangle$ is arbitrary, we have

$$[\hat{H}, \hat{U}(m,n)] = \big(E_m - E_n\big)\hat{U}(m,n).$$

(c) The product $\hat{U}(m,n)\hat{U}^\dagger(p,q)$ can be evaluated as follows

$$\begin{aligned}
\hat{U}(m,n)\hat{U}^\dagger(p,q) &= |\varphi_m\rangle\langle\varphi_n|\varphi_q\rangle\langle\varphi_p| \\
&= \delta_{nq}\,|\varphi_m\rangle\langle\varphi_p| \\
&= \delta_{nq}\hat{U}(m,p).
\end{aligned}$$

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

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

$$\begin{aligned}
\mathrm{Tr}\{\hat{U}(m,n)\} &= \sum_p \langle\varphi_p|\hat{U}(m,n)|\varphi_p\rangle \\
&= \sum_p \langle\varphi_p|\varphi_m\rangle\langle\varphi_n|\varphi_p\rangle \\
&= \sum_p \delta_{pm}\delta_{np} \\
&= \delta_{mn}.
\end{aligned}$$

Thus, $\mathrm{Tr}\{\hat{U}(m,n)\} = \delta_{mn}$.

(e) Making use of the closure relation of the eigenvectors of $\hat{H}$, we have

$$\begin{aligned}
\hat{A} &= 1\cdot\hat{A}\cdot 1 = \hat{P}_{\{\varphi_m\}}\hat{A}\hat{P}_{\{\varphi_n\}} \\
&= \sum_{mn} |\varphi_m\rangle\langle\varphi_m|\,\hat{A}\,|\varphi_n\rangle\langle\varphi_n| \\
&= \sum_{mn} |\varphi_m\rangle\, A_{mn}\,\langle\varphi_n| \\
&= \sum_{mn} A_{mn}\,|\varphi_m\rangle\langle\varphi_n| \\
&= \sum_{mn} A_{mn}\hat{U}(m,n).
\end{aligned}$$

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

(f) The trace $\mathrm{Tr}\{\hat{A}U^\dagger(p,q)\}$ can be evaluated as follows

$$\begin{aligned}
\mathrm{Tr}\{\hat{A}U^\dagger(p,q)\} &= \mathrm{Tr}\{\hat{A}\,|\varphi_q\rangle\langle\varphi_p|\} \\
&= \sum_n \langle\varphi_n|\hat{A}|\varphi_q\rangle\langle\varphi_p|\varphi_n\rangle \\
&= \sum_n A_{nq}\delta_{pn} \\
&= A_{pq}.
\end{aligned}$$

Thus, $A_{pq} = \mathrm{Tr}\{\hat{A}U^\dagger(p,q)\}$.

2. **[C-T Exercise 2-2]** In a three-dimensional vector space, consider the operator whose matrix, in an orthonormal basis $\{|1\rangle,|2\rangle,|3\rangle\}$, is written as $L_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$.

   (a) Is L_y Hermitian? Calculate its eigenvalues and eigenvectors (giving their normalized expansion in terms of the $\{|1\rangle,|2\rangle,|3\rangle\}$ basis).

   (b) Calculate the matrices which represent the projectors onto these eigenvectors. Then verify that they satisfy the orthogonality and closure relations.

(a) The transpose of L_y is

$$L_y^t = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix}.$$

The complex conjugate of L_y^t is given by

$$L_y^{t\,*} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

From the fact that the Hermitian conjugate of a matrix is equal to the complex conjugate of the transpose of the matrix, we have

$$L_y^\dagger = L_y^{t\,*} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

Comparing $L_y^\dagger$ with L_y, we see that $L_y^\dagger = L_y$. Therefore, L_y is Hermitian.
Let the eigenvalue of $\hat{L}_y$ be λ. Let the corresponding eigenvector be $|\varphi\rangle$ with

$$|\varphi\rangle = a\,|1\rangle + b\,|2\rangle + c\,|3\rangle\,.$$

In the column-matrix form, we have

$$\varphi = \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Eigenvalues of L_y. The matrix form of the eigenequation of L_y, $L_y\varphi = \lambda\varphi$, is given by

$$\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Performing the matrix product yields

$$\begin{aligned} -\lambda a \quad -i\frac{\hbar}{\sqrt{2}}b \qquad\qquad\quad &= 0, \\ i\frac{\hbar}{\sqrt{2}}a \quad -\lambda b \quad -i\frac{\hbar}{\sqrt{2}}c &= 0, \\ i\frac{\hbar}{\sqrt{2}}b \quad -\lambda c &= 0. \end{aligned}$$

The condition for the existence of nontrivial solutions of the above set of homogeneous linear equations for a, b, and c is

$$\begin{vmatrix} -\lambda & -i\frac{\hbar}{\sqrt{2}} & 0 \\ i\frac{\hbar}{\sqrt{2}} & -\lambda & -i\frac{\hbar}{\sqrt{2}} \\ 0 & i\frac{\hbar}{\sqrt{2}} & -\lambda \end{vmatrix} = 0.$$

Evaluating the determinant, we obtain

$$\lambda^3 - \hbar^2\lambda = 0$$

from which we obtain the following three eigenvalues of L_y

$$\lambda_1 = -\hbar,\ \lambda_2 = 0,\ \lambda_3 = \hbar.$$

To obtain the eigenvector corresponding to an eigenvalue, we insert the eigenvalue into the above-obtained equations for a, b, and c.

Eigenvector corresponding to $\lambda_1 = -\hbar$. Inserting $\lambda_1 = -\hbar$ into the equation for a, b, and c yields

$$\begin{aligned}
&\hbar a - i\frac{\hbar}{\sqrt{2}}b = 0,\\
&i\frac{\hbar}{\sqrt{2}}a + \hbar b - i\frac{\hbar}{\sqrt{2}}c = 0,\\
&i\frac{\hbar}{\sqrt{2}}b + \hbar c = 0
\end{aligned}$$

from which we obtain

$$b = -i\sqrt{2}\,a,\ \ c = -i\frac{1}{\sqrt{2}}b = -a.$$

Thus, in terms of a, the eigenfunction of L_y corresponding to the eigenvalue $\lambda_1 = -\hbar$ is given by

$$\varphi_1 = \begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix} a.$$

From the normalization condition $\varphi_1^\dagger \varphi_1 = 1$, we have

$$\begin{pmatrix} 1 & i\sqrt{2} & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix} |a|^2 = 1.$$

Evaluating the matrix product in the above equation yields $4|a|^2 = 1$. We thus have $|a| = 1/2$. We choose $a = 1/2$. The normalized wave function corresponding to the eigenvalue $\lambda_1 = -\hbar$ is given by

$$\varphi_1 = \frac{1}{2}\begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix}$$

The normalized expansion of φ_1 in terms of the $\{|1\rangle, |2\rangle, |3\rangle\}$ basis is given by

$$|\varphi_1\rangle = \frac{1}{2}\big(|1\rangle - i\sqrt{2}\,|2\rangle - |3\rangle\big).$$

Eigenvector corresponding to $\lambda_2 = 0$. Inserting $\lambda_2 = 0$ into the equation for a, b, and c yields

$$\begin{aligned}
b &= 0,\\
c &= a.
\end{aligned}$$

Thus, in terms of a, the eigenfunction of L_y corresponding to the eigenvalue $\lambda_2 = 0$ is given by

$$\varphi_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} a.$$

From the normalization condition $\varphi_2^\dagger \varphi_2 = 1$, we have

$$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} |a|^2 = 1.$$

Evaluating the matrix product in the above equation yields $2|a|^2 = 1$. We thus have $|a| = 1/\sqrt{2}$. We choose $a = 1/\sqrt{2}$. The normalized wave function corresponding to the eigenvalue $\lambda_2 = 0$ is given by

$$\varphi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

The normalized expansion of φ_2 in terms of the $\{|1\rangle, |2\rangle, |3\rangle\}$ basis is given by

$$|\varphi_2\rangle = \frac{1}{\sqrt{2}}\big(|1\rangle + |3\rangle\big).$$

Eigenvector corresponding to $\lambda_3 = \hbar$. Inserting $\lambda_3 = \hbar$ into the equation for a, b, and c yields

$$\begin{aligned}
&-\hbar a - i\frac{\hbar}{\sqrt{2}}b = 0,\\
&i\frac{\hbar}{\sqrt{2}}a - \hbar b - i\frac{\hbar}{\sqrt{2}}c = 0,\\
&i\frac{\hbar}{\sqrt{2}}b - \hbar c = 0
\end{aligned}$$

from which we obtain

$$b = i\sqrt{2}\,a,\ \ c = i\frac{1}{\sqrt{2}}b = -a.$$

Thus, in terms of a, the eigenfunction of L_y corresponding to the eigenvalue $\lambda_3 = \hbar$ is given by

$$\varphi_3 = \begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} a.$$

From the normalization condition $\varphi_3^\dagger \varphi_3 = 1$, we have

$$\begin{pmatrix} 1 & -i\sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} |a|^2 = 1.$$

Evaluating the matrix product in the above equation yields $4|a|^2 = 1$. We thus have $|a| = 1/2$. We choose $a = 1/2$. The normalized wave function corresponding to the eigenvalue $\lambda_3 = \hbar$ is given by

$$\varphi_3 = \frac{1}{2}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix}$$

The normalized expansion of φ_3 in terms of the $\{|1\rangle, |2\rangle, |3\rangle\}$ basis is given by

$$|\varphi_3\rangle = \frac{1}{2}\big(|1\rangle + i\sqrt{2}\,|2\rangle - |3\rangle\big).$$

In summary, we have obtained the following eigenvalues and eigenvectors of L_y in the orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle\}$

Eigenvalue	**Eigenfunction**	**Eigenvector**
$\lambda_1 = -\hbar$	$\varphi_1 = \frac{1}{2}\begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix}$	$\lvert\varphi_1\rangle = \frac{1}{2}\big(\lvert 1\rangle - i\sqrt{2}\,\lvert 2\rangle - \lvert 3\rangle\big)$
$\lambda_2 = 0$	$\varphi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$	$\lvert\varphi_2\rangle = \frac{1}{\sqrt{2}}\big(\lvert 1\rangle + \lvert 3\rangle\big)$
$\lambda_3 = \hbar$	$\varphi_3 = \frac{1}{2}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix}$	$\lvert\varphi_3\rangle = \frac{1}{2}\big(\lvert 1\rangle + i\sqrt{2}\,\lvert 2\rangle - \lvert 3\rangle\big)$

(b) The matrix representing the projector onto $|\varphi_1\rangle$ is given by

$$P_1 = \varphi_1\varphi_1^\dagger = \frac{1}{4}\begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix}\begin{pmatrix} 1 & i\sqrt{2} & -1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}.$$

The matrix representing the projector onto $|\varphi_2\rangle$ is given by

$$P_2 = \varphi_2\varphi_2^\dagger = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

The matrix representing the projector onto $|\varphi_3\rangle$ is given by

$$P_3 = \varphi_3\varphi_3^\dagger = \frac{1}{4}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix}.$$

The product P_1P_2 is given by

$$P_1P_2 = \frac{1}{8}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

The product P_2P_1 is also zero,

$$P_2P_1 = \frac{1}{8}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

The product P_2P_3 is given by

$$P_2P_3 = \frac{1}{8}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

The product P_3P_2 is also zero,

$$P_3P_2 = \frac{1}{8}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

The product P_3P_1 is given by

$$P_3P_1 = \frac{1}{16}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

The product P_1P_3 is also zero,

$$P_1P_3 = \frac{1}{16}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0.$$

Thus, the matrices representing the projectors onto the eigenvectors of L_y satisfy the orthogonality relation. The sum of P_1, P_2, and P_3 is given by

$$P_1 + P_2 + P_3 = \frac{1}{4}\begin{pmatrix} 1 & i\sqrt{2} & -1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ -1 & -i\sqrt{2} & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1 & -i\sqrt{2} & -1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, the sum of P_1, P_2, and P_3 is equal to a unit matrix. That is, the matrices representing the projectors onto the eigenvectors of L_y satisfy the closure relation.

3. **[C-T Exercise 2-3]** The state space of a certain physical system is three-dimensional. Let $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ be an orthonormal basis of this space. The kets $|\psi_0\rangle$ and $|\psi_1\rangle$ are defined by

$$
\begin{aligned}
|\psi_0\rangle &= \frac{1}{\sqrt{2}}\,|u_1\rangle + \frac{i}{2}\,|u_2\rangle + \frac{1}{2}\,|u_3\rangle, \\
|\psi_1\rangle &= \frac{1}{\sqrt{3}}\,|u_1\rangle + \frac{i}{\sqrt{3}}\,|u_3\rangle\,.
\end{aligned}
$$

(a) Are these kets normalized?

(b) Calculate the matrices ρ_0 and ρ_1 representing, in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis, the projection operators onto the state $|\psi_0\rangle$ and onto the state $|\psi_1\rangle$. Verify that these matrices are Hermitian.

(a) The square of the norm of $|\psi_0\rangle$ is given by

$$
\begin{aligned}
\langle\psi_0|\psi_0\rangle &= \left[\frac{1}{\sqrt{2}}\,\langle u_1| - \frac{i}{2}\,\langle u_2| + \frac{1}{2}\,\langle u_3|\right]\left[\frac{1}{\sqrt{2}}\,|u_1\rangle + \frac{i}{2}\,|u_2\rangle + \frac{1}{2}\,|u_3\rangle\right] \\
&= \left(\frac{1}{\sqrt{2}}\right)^2 + \left(-\frac{i}{2}\right)\left(\frac{i}{2}\right) + \left(\frac{1}{2}\right)^2 = 1.
\end{aligned}
$$

$\langle\psi_0|\psi_0\rangle = 1$ indicates that the norm of $|\psi_0\rangle$ is equal to unity. Thus, $|\psi_0\rangle$ is normalized. The square of the norm of $|\psi_1\rangle$ is given by

$$
\begin{aligned}
\langle\psi_1|\psi_1\rangle &= \left[\frac{1}{\sqrt{3}}\,\langle u_1| - \frac{i}{\sqrt{3}}\,\langle u_3|\right]\left[\frac{1}{\sqrt{3}}\,|u_1\rangle + \frac{i}{\sqrt{3}}\,|u_3\rangle\right] \\
&= \left(\frac{1}{\sqrt{3}}\right)^2 + \left(-\frac{i}{\sqrt{3}}\right)\left(\frac{i}{\sqrt{3}}\right) = \frac{2}{3}.
\end{aligned}
$$

Thus, $|\psi_1\rangle$ is not normalized. The normalized $|\psi_1\rangle$ is given by

$$
|\psi_1\rangle = \frac{1}{\sqrt{2}}\,|u_1\rangle + \frac{i}{\sqrt{2}}\,|u_3\rangle\,.
$$

The above normalized $|\psi_1\rangle$ will be used in the following calculations.

(b) The projection operator $\hat{\rho}_0$ is given by

$$
\begin{aligned}
\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0| &= \left[\frac{1}{\sqrt{2}}\,|u_1\rangle + \frac{i}{2}\,|u_2\rangle + \frac{1}{2}\,|u_3\rangle\right]\left[\frac{1}{\sqrt{2}}\,\langle u_1| - \frac{i}{2}\,\langle u_2| + \frac{1}{2}\,\langle u_3|\right] \\
&= \frac{1}{2}\,|u_1\rangle\langle u_1| - \frac{i}{2\sqrt{2}}\,|u_1\rangle\langle u_2| + \frac{1}{2\sqrt{2}}\,|u_1\rangle\langle u_3| \\
&\quad + \frac{i}{2\sqrt{2}}\,|u_2\rangle\langle u_1| + \frac{1}{4}\,|u_2\rangle\langle u_2| + \frac{i}{4}\,|u_2\rangle\langle u_3| \\
&\quad + \frac{1}{2\sqrt{2}}\,|u_3\rangle\langle u_1| - \frac{i}{4}\,|u_3\rangle\langle u_2| + \frac{1}{4}\,|u_3\rangle\langle u_3|\,.
\end{aligned}
$$

From the above expression, we can easily infer the matrix representing $\hat{\rho}_0$. We have

$$
\rho_0 = \begin{pmatrix}
\frac{1}{2} & -\frac{i}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\
\frac{i}{2\sqrt{2}} & \frac{1}{4} & \frac{i}{4} \\
\frac{1}{2\sqrt{2}} & -\frac{i}{4} & \frac{1}{4}
\end{pmatrix}.
$$

From the above matrix representing $\hat{\rho}_0$, we see that ρ_0 is a Hermitian matrix.

The projection operator $\hat{\rho}_1$ is given by

$$\hat{\rho}_1 = |\psi_1\rangle\langle\psi_1| = \left[\ \frac{1}{\sqrt{2}}\,|u_1\rangle + \frac{i}{\sqrt{2}}\,|u_3\rangle\ \right]\left[\ \frac{1}{\sqrt{2}}\,\langle u_1| - \frac{i}{\sqrt{2}}\,\langle u_3|\ \right]$$
$$= \frac{1}{2}\,|u_1\rangle\langle u_1| - \frac{i}{2}\,|u_1\rangle\langle u_3| + \frac{i}{2}\,|u_3\rangle\langle u_1| + \frac{1}{2}\,|u_3\rangle\langle u_3|\,.$$

From the above expression, we can easily infer the matrix representing $\hat{\rho}_1$. We have

$$\rho_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 1 \end{pmatrix}$$

From the above matrix representing $\hat{\rho}_1$, we see that ρ_1 is a Hermitian matrix.
Let us check the properties of ρ_0 and ρ_1. For ρ_0^2, we have

$$\rho_0^2 = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{i}{2\sqrt{2}} & \frac{1}{4} & \frac{i}{4} \\ \frac{1}{2\sqrt{2}} & -\frac{i}{4} & \frac{1}{4} \end{pmatrix}\begin{pmatrix} \frac{1}{2} & -\frac{i}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{i}{2\sqrt{2}} & \frac{1}{4} & \frac{i}{4} \\ \frac{1}{2\sqrt{2}} & -\frac{i}{4} & \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{i}{2\sqrt{2}} & \frac{1}{4} & \frac{i}{4} \\ \frac{1}{2\sqrt{2}} & -\frac{i}{4} & \frac{1}{4} \end{pmatrix} = \rho_0.$$

For ρ_1^2, we have

$$\rho_1^2 = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{i}{2} \\ 0 & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} \end{pmatrix}\begin{pmatrix} \frac{1}{2} & 0 & -\frac{i}{2} \\ 0 & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{i}{2} \\ 0 & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} \end{pmatrix} = \rho_1.$$

Thus, ρ_0 and ρ_1 indeed possess the property of projection operators that the square of a projection operator is equal to itself.

4. **[C-T Exercise 2-9]** Let $\hat{H}$ be the Hamiltonian operator of a physical system. Denote by $|\varphi_n\rangle$ the eigenvectors of $\hat{H}$, with eigenvalues E_n, $\hat{H}\,|\varphi_n\rangle = E_n\,|\varphi_n\rangle$.

   (a) For an arbitrary operator $\hat{A}$, prove the relation $\langle\varphi_n|[\hat{A},\hat{H}]|\varphi_n\rangle = 0$.

   (b) Consider a one-dimensional problem, where the physical system is a particle of mass m and of potential energy $\hat{V}(\hat{x})$. In this case, $\hat{H}$ is written as $\hat{H} = \dfrac{1}{2m}\hat{p}^2 + \hat{V}(\hat{x})$.

      i. In terms of $\hat{p}$, $\hat{x}$, and $\hat{V}(\hat{x})$, find the commutators: $[\hat{H},\hat{p}]$, $[\hat{H},\hat{x}]$, and $[\hat{H},\hat{x}\hat{p}]$.

      ii. Show that the matrix element $\langle\varphi_n|\hat{p}|\varphi_n\rangle$ is zero.

      iii. Establish a relation between $E_k = \langle\varphi_n|\dfrac{\hat{p}^2}{2m}|\varphi_n\rangle$ and $\langle\varphi_n|\hat{x}\dfrac{d\hat{V}(\hat{x})}{d\hat{x}}|\varphi_n\rangle$. Apply the derived relation to $\hat{V}(\hat{x}) = V_0\hat{x}^\lambda$ with $\lambda = 2, 4, 6, \cdots$ and $V_0 > 0$.

(a) For $\langle\varphi_n|[\hat{A},\ \hat{H}]|\varphi_n\rangle$, we have

$$\langle\varphi_n|[\hat{A},\ \hat{H}]|\varphi_n\rangle = \langle\varphi_n|\hat{A}\hat{H} - \hat{H}\hat{A}|\varphi_n\rangle\,.$$

Making use of $\hat{H}\,|\varphi_n\rangle = E_n\,|\varphi_n\rangle$ and $\langle\varphi_n|\,\hat{H} = E_n\,\langle\varphi_n|$, we have

$$\langle\varphi_n|[\hat{A},\ \hat{H}]|\varphi_n\rangle = \langle\varphi_n|\hat{A}E_n - E_n\hat{A}|\varphi_n\rangle = E_n\big[\,\langle\varphi_n|\hat{A}|\varphi_n\rangle - \langle\varphi_n|\hat{A}|\varphi_n\rangle\,\big] = 0.$$

(b) i. In the form of a power series, $\hat{V}(\hat{x})$ is given by

$$\hat{V}(\hat{x}) = \sum_{n=0}^{\infty} \frac{V^{(n)}(0)}{n!} \hat{x}^n$$

The commutator $[\hat{H},\ \hat{p}]$ is given by

$$[\hat{H},\ \hat{p}] = [\hat{V}(\hat{x}),\ \hat{p}] = \sum_{n=0}^{\infty} \frac{V^{(n)}(0)}{n!} [\hat{x}^n,\ \hat{p}].$$

The commutator $[\hat{x}^n,\ \hat{p}]$ can be evaluated through repeatedly using $[\hat{A}\hat{B},\ \hat{C}] = \hat{A}[\hat{B},\ \hat{C}] + [\hat{A},\ \hat{C}]\hat{B}$ and $[\hat{x}, \hat{p}] = i\hbar$. We have

$$\begin{aligned}
[\hat{x}^n,\ \hat{p}] &= [\hat{x}^{n-1}\hat{x},\ \hat{p}] = \hat{x}^{n-1}[\hat{x},\ \hat{p}] + [\hat{x}^{n-1},\ \hat{p}]\hat{x} = i\hbar\hat{x}^{n-1} + [\hat{x}^{n-1},\ \hat{p}]\hat{x} \\
&= i\hbar\hat{x}^{n-1} + [\hat{x}^{n-2}\hat{x},\ \hat{p}]\hat{x} = i\hbar\hat{x}^{n-1} + \hat{x}^{n-2}[\hat{x},\ \hat{p}]\hat{x} + [\hat{x}^{n-2},\ \hat{p}]\hat{x}^2 \\
&= 2i\hbar\hat{x}^{n-1} + [\hat{x}^{n-2},\ \hat{p}]\hat{x}^2 \\
&= \cdots \\
&= ni\hbar\hat{x}^{n-1}.
\end{aligned}$$

The commutator $[\hat{H},\ \hat{p}]$ is then given by

$$[\hat{H},\ \hat{p}] = \sum_{n=0}^{\infty} \frac{V^{(n)}(0)}{n!} \cdot ni\hbar\hat{x}^{n-1} = i\hbar \sum_{n=1}^{\infty} \frac{V^{(n)}(0)}{(n-1)!} \hat{x}^{n-1} = i\hbar \frac{d\hat{V}(\hat{x})}{d\hat{x}}.$$

The commutator $[\hat{H},\ \hat{x}]$ can be evaluated as follows

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

Making use of the above-obtained results for $[\hat{H},\ \hat{x}]$ and $[\hat{H},\ \hat{p}]$, we can easily evaluate the commutator $[\hat{H},\ \hat{x}\hat{p}]$. We have

$$\begin{aligned}
[\hat{H},\ \hat{x}\hat{p}] &= \hat{x}[\hat{H},\ \hat{p}] + [\hat{H},\ \hat{x}]\hat{p} \\
&= i\hbar\hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}} - \frac{i\hbar}{m}\hat{p}^2 \\
&= -i\hbar\left[\, 2\frac{\hat{p}^2}{2m} - \hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}} \,\right].
\end{aligned}$$

ii. From the above-obtained result

$$[\hat{H},\ \hat{x}] = -\frac{i\hbar}{m}\hat{p},$$

we have

$$\hat{p} = \frac{im}{\hbar}[\hat{H},\ \hat{x}].$$

The matrix element $\langle\varphi_n|\hat{p}|\varphi_n\rangle$ can be then written as

$$\langle\varphi_n|\hat{p}|\varphi_n\rangle = \frac{im}{\hbar}\langle\varphi_n|[\hat{H},\ \hat{x}]|\varphi_n\rangle.$$

Utilizing $\langle\varphi_n|[\hat{A}, \hat{H}]|\varphi_n\rangle = 0$ with $\hat{A} = \hat{x}$, we have

$$\langle\varphi_n|\hat{p}|\varphi_n\rangle = 0.$$

iii. Making use of the above-obtained result

$$[\hat{H},\ \hat{x}\hat{p}] = -i\hbar\left[\,2\frac{\hat{p}^2}{2m} - \hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}}\,\right],$$

the matrix element $\langle\varphi_n|[\hat{H},\ \hat{x}\hat{p}]|\varphi_n\rangle$ is given by

$$\langle\varphi_n|[\hat{H},\ \hat{x}\hat{p}]|\varphi_n\rangle = -i\hbar\,\langle\varphi_n|\left[\,2\frac{\hat{p}^2}{2m} - \hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}}\,\right]|\varphi_n\rangle\,.$$

Utilizing $\langle\varphi_n|[\hat{A},\hat{H}]|\varphi_n\rangle = 0$ with $\hat{A} = \hat{x}\hat{p}$, we have

$$\langle\varphi_n|\left[\,2\frac{\hat{p}^2}{2m} - \hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}}\,\right]|\varphi_n\rangle = 0.$$

That is,

$$2E_k = \langle\varphi_n|2\frac{\hat{p}^2}{2m}|\varphi_n\rangle = \langle\varphi_n|\hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}}|\varphi_n\rangle\,.$$

The above equation is the mathematical statement of the virial theorem.
For $\hat{V}(\hat{x}) = V_0\hat{x}^\lambda$ with $\lambda = 2, 4, 6, \cdots$ and $V_0 > 0$, we have

$$\hat{x}\frac{d\hat{V}(\hat{x})}{d\hat{x}} = \hat{x}\cdot\lambda V_0\hat{x}^{\lambda-1} = \lambda V_0\hat{x}^\lambda = \lambda\hat{V}(\hat{x}).$$

Thus,

$$2E_k = \lambda\,\langle\varphi_n|\hat{V}(\hat{x})|\varphi_n\rangle = \lambda\overline{V},$$

where $\overline{V} = \langle\varphi_n|\hat{V}(\hat{x})|\varphi_n\rangle$ is the average of the potential energy.
Note that, for $\lambda = 2$, we have

$$E_k = \overline{V}.$$

That is, for a particle in a stationary state of a harmonic potential, the average of its kinetic energy is equal to the average of its potential energy.

5. **[C-T Exercise 2-10]** Using the relation $\langle x|p\rangle = (2\pi\hbar)^{-1/2}e^{ipx/\hbar}$, find the expressions of $\langle x|\hat{x}\hat{p}|\psi\rangle$ and $\langle x|\hat{p}\hat{x}|\psi\rangle$ in terms of $\psi(x)$. Can these results be found directly by using the fact that in the $\{|x\rangle\}$ representation, $\hat{p}$ acts like $-i\hbar\dfrac{d}{dx}$?

Evaluation of $\langle x|\hat{x}\hat{p}|\psi\rangle$.

[Method I.] Making use of $\langle x|\hat{x}|\varphi\rangle = x\,\langle x|\varphi\rangle$, we have

$$\langle x|\hat{x}\hat{p}|\psi\rangle = x\,\langle x|\hat{p}|\psi\rangle\,.$$

Making use of the magic one

$$\int dp\ \ |p\rangle\langle p| = 1,$$

we have

$$\langle x|\hat{x}\hat{p}|\psi\rangle = x\int dp\ \ \langle x|p\rangle\langle p|\hat{p}|\psi\rangle\,.$$

Making use of $\langle p|\hat{p}|\psi\rangle = p\,\langle p|\psi\rangle$, we have

$$\langle x|\hat{x}\hat{p}|\psi\rangle = x\int dp\; p\,\langle x|p\rangle\langle p|\psi\rangle\,.$$

Making use of the magic one

$$\int dx' \;\; |x'\rangle\langle x'| = 1,$$

we have

$$\langle x|\hat{x}\hat{p}|\psi\rangle = x\int dx' \int dp \; p \, \langle x|p\rangle\langle p|x'\rangle\langle x'|\psi\rangle \, .$$

Making use of $\langle x'|\psi\rangle = \psi(x')$ and

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}, \; \langle p|x'\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx'/\hbar},$$

we have

$$\begin{aligned}
\langle x|\hat{x}\hat{p}|\psi\rangle &= x\int dx' \int dp \; p\frac{1}{2\pi\hbar}e^{ip(x-x')/\hbar}\psi(x') \\
&= i\hbar x\int dx' \int dp \; \frac{1}{2\pi\hbar}\frac{de^{ip(x-x')/\hbar}}{dx'}\psi(x') \\
&= -i\hbar x\int dx' \int dp \; \frac{1}{2\pi\hbar}e^{ip(x-x')/\hbar}\frac{d\psi(x')}{dx'} \\
&= -i\hbar x\int dx' \; \delta(x-x')\frac{d\psi(x')}{dx'} \\
&= -i\hbar x\frac{d\psi(x)}{dx}.
\end{aligned}$$

[Method II.] The above result can be also obtained by making use of

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\,\langle x|\psi\rangle = -i\hbar\frac{d\psi(x)}{dx}.$$

We have

$$\langle x|\hat{x}\hat{p}|\psi\rangle = x\,\langle x|\hat{p}|\psi\rangle = -i\hbar x\frac{d\psi(x)}{dx}.$$

Evaluation of $\langle x|\hat{p}\hat{x}|\psi\rangle$.

[Method I.] Making use of the fundamental commutation relation in quantum mechanics, $[\hat{x},\;\hat{p}] = i\hbar$, we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = -i\hbar\,\langle x|\psi\rangle + \langle x|\hat{x}\hat{p}|\psi\rangle = -i\hbar\psi(x) + \langle x|\hat{x}\hat{p}|\psi\rangle \, .$$

Making use of the above-obtained result

$$\langle x|\hat{x}\hat{p}|\psi\rangle = -i\hbar x\frac{d\psi(x)}{dx},$$

we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = -i\hbar\psi(x) - i\hbar x\frac{d\psi(x)}{dx}.$$

[Method II.] In this method, we use the magic ones to evaluate $\langle x|\hat{x}\hat{p}|\psi\rangle$. Making use of the magic one

$$\int dp \;\; |p\rangle\langle p| = 1,$$

we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = \int dp \;\; \langle x|p\rangle\langle p|\hat{p}\hat{x}|\psi\rangle$$

Making use of $\langle p|\hat{p}|\varphi\rangle = p\,\langle p|\varphi\rangle$, we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = \int dp\; p\,\langle x|p\rangle\langle p|\hat{x}|\psi\rangle\,.$$

Making use of the magic one

$$\int dx' \;\; |x'\rangle\langle x'| = 1,$$

we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = \int dx' \int dp\; p\,\langle x|p\rangle\langle p|x'\rangle\langle x'|\hat{x}|\psi\rangle\,.$$

Making use of $\langle x'|\hat{x}|\psi\rangle = x'\,\langle x'|\psi\rangle$, we have

$$\begin{aligned}
\langle x|\hat{p}\hat{x}|\psi\rangle &= \int dx'\; x' \int dp\; p\,\langle x|p\rangle\langle p|x'\rangle\langle x'|\psi\rangle = \int dx'\; x' \int dp\; p\,\langle x|p\rangle\langle p|x'\rangle\,\psi(x') \\
&= \int dx'\; x' \int dp\; p \frac{1}{2\pi\hbar} e^{ip(x-x')/\hbar}\psi(x') = i\hbar \int dx'\; x' \int dp\; \frac{1}{2\pi\hbar}\frac{de^{ip(x-x')/\hbar}}{dx'}\psi(x') \\
&= -i\hbar \int dx' \;\int dp\; \frac{1}{2\pi\hbar} e^{ip(x-x')/\hbar}\frac{d[x'\psi(x')]}{dx'} = -i\hbar \int dx'\; \delta(x-x')\frac{d[x'\psi(x')]}{dx'} \\
&= -i\hbar\frac{d[x\psi(x)]}{dx} = -i\hbar\psi(x) - i\hbar x\frac{d\psi(x)}{dx}.
\end{aligned}$$

[Method III.] In this method, we utilize

$$\langle x|\hat{p}|\varphi\rangle = -i\hbar\frac{d}{dx}\,\langle x|\varphi\rangle,$$

we have

$$\langle x|\hat{p}\hat{x}|\psi\rangle = -i\hbar\frac{d}{dx}\,\langle x|\hat{x}|\psi\rangle = -i\hbar\frac{d}{dx}\big(x\,\langle x|\psi\rangle\big) = -i\hbar\frac{d}{dx}\big[x\psi(x)\big] = -i\hbar\psi(x) - i\hbar x\frac{d\psi(x)}{dx}.$$