I Illustrative Examples

Three Hamiltonians that are useful for illustrations :

- Particle in a box.
- Simple harmonic oscillator.
- Two-state system.

1. Particle in a box :

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$ where $V(\hat{x}) = 0$ for $x \in (0, L)$ and ∞ otherwise.

The eigenvector and eigenvalues of $\hat{H}$ are given by :

$$\langle x | E_n \rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \equiv \frac{n^2 \pi^2}{2mL^2}$$

($\hbar = 1$ notation)

with $n = 1, 2, \ldots, \infty$.

The Hilbert space $\mathcal{H}$ is infinite dimensional. One choice of basis for $\mathcal{H}$ is $|x\rangle$ with $x \in (0, L)$. Another possible basis is $|E_n\rangle$ with $n = 1, 2, -- \infty$. There exist infinitely many other possibilities for the basis!

<u>Example:</u> A particle in a box is in its ground state. A measurement is made of its position. What is the probability that the outcome lies in the window $x \in [0, \frac{L}{3}]$.

Intuitively, probability $= \int_0^{L/3} |\langle x|E_1\rangle|^2 dx$

but let's re-derive it more formally.

Projection P onto the measurement subspace $= \int_0^{L/3} |x\rangle\langle x| \, dx$

$$\text{Probability} = \langle E_1 | P \; P | E_1 \rangle$$

$$= \langle E_1 | P | E_1 \rangle \qquad (P^2 = P)$$

$$= \int_0^{L/3} \langle E_1 | x \rangle \langle x | E_1 \rangle \, dx$$

$$= \int_0^{L/3} | \langle E_1 | x \rangle |^2 \, dx .$$

$$= \int_0^{L/3} \frac{2}{L} \sin^2\left(\frac{\pi x}{L}\right) dx$$

<u>Example:</u> A particle is in a two dimensional square shaped box of size $L \times L$.

A measurement is made of its energy.

What is the probability that the outcome is $\dfrac{5\pi^2}{2mL^2}$?

2. Simple harmonic oscillator:

(Gottfried, 4.2)

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

Let's rescale: $x\sqrt{m\omega^2} \to x$

$p/\sqrt{m} \to p$.

so that $H = \frac{p^2}{2} + \frac{x^2}{2}$.

Define $a = \frac{x+ip}{\sqrt{2}}$, $a^+ = \frac{x-ip}{\sqrt{2}}$.

$\Rightarrow \quad H = a^+ a + \frac{1}{2}$, with $[a, a^+] = 1$.

Importantly, $a^+ a$ is a <u>positive-definite</u> operator, i.e., for any state $|\varphi\rangle$,

$\langle\varphi| a^+ a |\varphi\rangle \geq 0 \Rightarrow$ eigenvalues of $a^+ a$ are <u>non-negative</u>. Our task is to find these eigenvalues.

Let's consider one specific eigenvector of $a^\dagger a$ with eigenvalue n (which is as yet undetermined). Let's denote this eigenvector as $|n\rangle$.

$$\Rightarrow \quad a^\dagger a \, |n\rangle = n \, |n\rangle .$$

Now consider $a|n\rangle$. We claim that this is also an eigenvector of $a^\dagger a$. To see this:

$$a^\dagger a \; a|n\rangle = (a a^\dagger - 1) \, a|n\rangle$$

$$= a \; a^\dagger a|n\rangle - a|n\rangle$$

$$= a \; n|n\rangle - a|n\rangle = (n-1) \, a|n\rangle .$$

$\Rightarrow$ $a|n\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $n-1$.

One can similarly show that $a^\dagger|n\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $n+1$.

Thus, $a|n\rangle \propto |n-1\rangle$, $a^+|n\rangle \propto |n+1\rangle$.

Let's find the proportionality constants.

We chose the convention that all eigenvectors are unit norm i.e.

$\langle n|n\rangle = 1 \;\; \forall n$.

$\Rightarrow$ if $a|n\rangle = c|n\rangle$

$\Rightarrow \langle n|\, a^+ a|n\rangle = |c|^2 \langle n|n\rangle$

$\Rightarrow n = |c|^2$

$\Rightarrow c = \sqrt{n}$ upto an irrelevant phase.

$\Rightarrow a|n\rangle = \sqrt{n}\,|n-1\rangle$

Similarly, $a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$.

Now, we use the constraint that a^+a is positive-definite. If n is not an integer, then one will generate eigenvectors of a^+a with negative eigenvalues.

for example $a|n = 0.4\rangle = \sqrt{0.4}\,|-0.6\rangle$ which is not allowed. On the other hand, if we restrict n to be integers, then eigenvectors with negative eigenvalues are not generated.

$$a|1\rangle = |0\rangle$$

$$a|0\rangle = 0\,|-1\rangle = 0.$$

Therefore, for consistency, we require $n \in$ non-negative integers.

$$\Rightarrow \quad H|n\rangle = (a^{+}a + \tfrac{1}{2})|n\rangle$$

$$= (n + \tfrac{1}{2})|n\rangle$$

$n = 0, 1, 2, \ldots \infty.$

Let's find real-space wave-fns. of SHO.

Ground state wave-fn. = $\langle x | n=0 \rangle$.

$$a | n=0 \rangle = 0$$

$$\Rightarrow (x + ip) | n=0 \rangle = 0$$

$$\Rightarrow \left(x + \frac{d}{dx}\right) | n=0 \rangle = 0$$

$$\Rightarrow x \langle x | n=0 \rangle + \frac{d}{dx} \langle x | n=0 \rangle = 0$$

$$\Rightarrow \langle x | n=0 \rangle \propto e^{-x^2/2}$$

Restoring physical units and normalizing

$$\langle x | n=0 \rangle = \left(\frac{m\omega}{\pi}\right)^{1/4} e^{-\frac{x^2 m\omega}{2}}$$

Using $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle$, one may construct real-space wave-fns for any $|n\rangle$. They turn out to be related to Hermite polynomials. See Gottfried 4.2.

— Quantum systems with finite Hilbert space

For particle in a box, $\mathcal{H}$ is infinite-dim. (basis $\{|x\rangle\}$ is infinite dimensional).

Far simpler are problems with a finite-dim $\mathcal{H}$. Let's consider a few examples.

(a) Consider $\mathcal{H}$ spanned by two states that we denote by $|0\rangle$ and $|1\rangle$. An arbitrary state is given by $c_1|0\rangle + c_2|1\rangle$ where c_1, c_2 are complex no's with $|c_1|^2 + |c_2|^2 = 1$.

An arbitrary operator $\hat{A}$ is fully specified by its action on the basis states:

$$\hat{A}|0\rangle = \langle 1|\hat{A}|0\rangle\, |1\rangle + \langle 0|\hat{A}|0\rangle\, |0\rangle$$

$$\hat{A}|1\rangle = \langle 1|\hat{A}|1\rangle\, |1\rangle + \langle 0|\hat{A}|1\rangle\, |1\rangle.$$

Thus the matrix representation of $\hat{A}$ in this basis is :

$$\hat{A} \equiv \begin{bmatrix} \langle 0|\hat{A}|0\rangle & \langle 0|\hat{A}|1\rangle \\ \\ \langle 1|\hat{A}|0\rangle & \langle 1|\hat{A}|1\rangle \end{bmatrix}$$

Change of basis :

There exist infinitely many possibilities for choosing basis. For example, another possibility is $|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$,

$|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$. Note that $\langle +|+\rangle$ $= \langle -|-\rangle = 1$ and $\langle +|-\rangle = 0$.

As a matrix equation, one may write

$$\begin{bmatrix} |+\rangle \\ |-\rangle \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}}_{U}\begin{bmatrix} |0\rangle \\ |1\rangle \end{bmatrix}.$$

One notices that $U^{+}U = \mathbb{1}$. This is a general property of matrix that implements a basis change, as it guarantees that the new basis is complete and orthonormal. For example, if the original basis is $\{|i\rangle\}$ and new basis is $\{|\alpha\rangle\}$, related as

$$|\alpha\rangle = \sum_i U_{\alpha i} |i\rangle \quad , \text{ then}$$

$$\langle \alpha | \beta \rangle = \sum_{ij} U^*_{\alpha i} \langle i| \; U_{\beta j} |j\rangle$$

$$= \quad U^*_{\alpha i} \; U_{\beta i}$$

$$= \sum_i U_{\beta i} (U^{+})_{i\alpha} = (UU^{+})_{\beta\alpha}$$

$$= \delta_{\alpha\beta}$$

The matrix representation of an operator $\hat{A}$ in the new basis is given by:

$$\tilde{\hat{A}}_{\alpha\beta} = \langle \alpha | \hat{A} | \beta \rangle$$

$$= \mathcal{U}^*_{\alpha i} \langle i | \hat{A} | j \rangle \mathcal{U}_{\beta j}$$

$$= \left(\mathcal{U} A \mathcal{U}^\dagger \right)_{\beta\alpha}$$

where A (without hat) denotes the matrix representation of $\hat{A}$ in the original basis $|i\rangle$.

Consider, for example the operator with matrix representation $\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$ in the basis $|0\rangle, |1\rangle$. In the new basis $|+\rangle, |-\rangle$, this same operator will now be represented as

$$\mathcal{U} \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} \mathcal{U}^\dagger$$ where

$\mathcal{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ as written above.

Calculations such as above can be done rather quickly by utilizing properties of Pauli matrices,

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$X^2 = Y^2 = Z^2 = \mathbb{1}$ X, Y, Z hermitian and unitary. Eigenvalues ± 1. They all anticommute $XY = iZ = -YX$ etc.

Eigenvectors :

$$X \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad X \begin{bmatrix} 1 \\ -1 \end{bmatrix} = -\begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

$$Y \begin{bmatrix} 1 \\ i \end{bmatrix} = \begin{bmatrix} 1 \\ i \end{bmatrix}, \quad Y \begin{bmatrix} 1 \\ -i \end{bmatrix} = -\begin{bmatrix} 1 \\ i \end{bmatrix}.$$

$$Z \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad Z \begin{bmatrix} 0 \\ 1 \end{bmatrix} = -\begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Lets return to the calculation of UAU^{+}

where $A = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} = Z$,

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}}(X+Z)$$

$$\Rightarrow UAU^{+} = \frac{1}{2}(X+Z)\,Z\,(X+Z)$$

$$= \frac{1}{2}[XZX + XZZ + ZZX + ZZZ]$$

$$= \frac{1}{2}[-Z + X + X + Z]$$

$$= X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Thus, the operator $\hat{A}$ in the basis $|0\rangle, |1\rangle$ is $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = Z$ and in the basis $|+\rangle, |-\rangle$ is $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = X$.

Note that the trace and determinant are unchanged after the basis change.

Problem: Lets chose the basis states $|0\rangle$, $|1\rangle$ so that $Z|0\rangle = |0\rangle$, $Z|1\rangle = -|1\rangle$. Consider the time-evolution of the state $|0\rangle$ by the following unitary U

$$|0\rangle \longrightarrow U|0\rangle$$

where $U = Z\left(\frac{X+Z}{\sqrt{2}}\right)\frac{(X-Y)}{\sqrt{2}}$.

In the final state, consider measuring the operator X. What is the probability of finding the outcome $+1$?

$$U = \frac{1}{2} Z(X+Z)(X-Y) = \frac{1}{2}[1+ZX][X-Y]$$

$$= \frac{1}{2}[X-Y+Z-i] = \frac{1}{2}\begin{bmatrix} 1-i & 1+i \\ 1-i & -1-i \end{bmatrix}$$

$$U^{\dagger}U = \frac{1}{4}\begin{bmatrix} 1+i & 1+i \\ 1-i & -1+i \end{bmatrix}\begin{bmatrix} 1-i & 1+i \\ 1-i & -1-i \end{bmatrix}$$

$$= \frac{1}{4}\begin{bmatrix} 2+2 & 0 \\ 0 & 2+2 \end{bmatrix} = 1$$

Prob. (outcome = +1)

$$= \left| \langle + | \; U \; | 0 \rangle \right|^2$$

$$= \frac{1}{4} \left| \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1-i & 1+i \\ 1-i & -1-i \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right|^2$$

$$= \frac{1}{4} \left| \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1-i \\ 1-i \end{bmatrix} \right|^2$$

$$= \frac{1}{4} \; |1-i|^2 \times 2 = 1.$$