2|9|2025 Day 15. Matrix Representation of states and Operators

Gram-Schmidt Orthogonalization:

Suppose we are given a set of N L.I. vectors $\{|u_i\rangle\}_{i=1,N}$ which are not necessarily orthogonal but, say, normalized.

i.e. $\langle u_i|u_i\rangle = 1 \; \forall i$

$\langle u_i|u_j\rangle \neq 0 \; \forall i \neq j$

Then we can come up with a set of O/N vectors from these. One procedure to do so is outlined below.

Let $|v_1\rangle = |u_1\rangle$ — (1)

define $|w_2\rangle \equiv |u_2\rangle - |v_1\rangle\langle v_1|u_2\rangle$ — (2)

Note that

$$\langle v_1|w_2\rangle = \langle v_1|u_2\rangle - \langle v_1|v_1\rangle \cdot \langle v_1|u_2\rangle$$

$(\because \langle v_1|v_1\rangle = 1)$ $= 0$ — (3)

$\therefore$ $|w_2\rangle$ is orthogonal to $|v_1\rangle$
We can normalize it to define the next vector in the list as

$$|v_2\rangle \equiv \frac{|w_2\rangle}{\sqrt{\langle w_2|w_2\rangle}} \quad -④$$

Now, let $$|w_3\rangle \equiv |u_3\rangle - \sum_{j=1}^{2} |v_j\rangle\langle v_j|u_3\rangle \quad ⑤$$

It's easily seen that

$$\langle v_1|w_3\rangle = \langle v_2|w_3\rangle = 0 \quad -⑥$$

Normalizing $|w_3\rangle$ we get the 3rd vector in our O/N list

$$|v_3\rangle \equiv |w_3\rangle \Big/ \sqrt{\langle w_3|w_3\rangle} \quad -⑦$$

In general, given ①, we can summarize the procedure as follows:

0. $|v_1\rangle \equiv |u_1\rangle$

1. $|w_{i+1}\rangle \equiv |u_{i+1}\rangle - \sum_{j=1}^{i} |v_j\rangle\langle v_j|u_{i+1}\rangle$

2. $|v_{i+1}\rangle \equiv |w_{i+1}\rangle \Big/ \sqrt{\langle w_{i+1}|w_{i+1}\rangle}$

$i = 1, N-1$

(8)

This procedure generates the O/N set $\{|v_i\rangle\}_{i=1,N}$ which spans the $\mathcal{H}$..

Suppose we are given a complete set of (L.I.) states parameterised by K real numbers $\lambda_1, \lambda_2 \cdots \lambda_K$..

$\rightarrow \{|\lambda_1 \lambda_2 \cdots \lambda_K\rangle\}$

$\therefore$ any state in the $\mathcal{H}$ can be written in terms of these.

$$|\Psi\rangle = \sum_{\lambda_1 \lambda_2 \cdots \lambda_K} |\lambda_1 \cdots \lambda_K\rangle\langle\lambda_1 \cdots \lambda_K|\Psi\rangle \quad (9)$$

The coefficients $\{\langle \lambda_1 \cdots \lambda_k | \Psi \rangle\}$ are then said to "represent" $|\Psi\rangle$.

The set $\{\langle \lambda_1 \cdots \lambda_k |\}$ is said to form a "representation" on $\mathcal{H}$.

We can generate another representation from these as

$$\langle \lambda_1 \lambda_2 \cdots \lambda_k | \longrightarrow \lambda_1 \langle \lambda_1 \lambda_2 \cdots \lambda_k | \quad -(10)$$

because these are also L.I.

(10) is a linear map and can be captured through the action of a linear operator $\hat{\lambda}_1$:

$$\langle \lambda_1 \cdots \lambda_k | \hat{\lambda}_1 = \lambda_1 \langle \lambda_1 \cdots \lambda_k | \quad -(11)$$

This is just an eigenvalue equation for the operator $\hat{\lambda}_1$, which is Hermitian owing to the reality of λ_1.

The same can be shown with all the real parameters, thereby realising the mutually compatible Hermitian operators $\{\hat{\lambda}_1, \hat{\lambda}_2 \ldots \hat{\lambda}_k\}$.

These are all observables since, by assumption, they lead to a complete set of states.

Hence, a representation parametrised by real numbers is actually a set of simultaneous eigenbras of a set of mutually compatible observables.

Now, since we have only used the eigenvalues to parametrise the states, there are 2 possibilities

1. Each set $(\lambda_1 \cdots \lambda_k)$ corresponds to a unique eigenbra in the complete set. Then, $\{\langle \lambda_1 \lambda_2 \ldots \lambda_k |\}$ are orthogonal.

In this case, $\{\hat{\lambda}_1, \hat{\lambda}_2, \dots \hat{\lambda}_k\}$ are said to form a <u>complete set of compatible observables</u>.

2. Some combinations of $\lambda_1, \lambda_2 \cdots \lambda_K$ do not lead to a unique state in the representation. For instance, let us say that including one more real parameter, μ_1, allows us to distinguish these (degenerate) states i.e. $\{\langle \lambda_1 \lambda_2 \cdots \lambda_K \mu_1 |\}$ are unique.

Then, as before, we can define another representation where these states are replaced by

$$\{\mu_1 \langle \lambda_1 \lambda_2 \cdots \lambda_K \mu_1 |\}$$

Since it is a linear map we have that $\exists$ an observable $\hat{\mu}_1$ s.t.

$$\langle \lambda_1 \lambda_2 \cdots \lambda_k \mu_1 | \hat{\mu}_1 = \mu_1 \langle \lambda_1 \lambda_2 \cdots \lambda_k \mu_1 | \quad -(12)$$

$\Rightarrow$ we found another compatible observable, $\hat{\mu}_1$, to complete the set.

The set $\{\langle \lambda_1 \lambda_2 \cdots \lambda_k \mu_1 |\}$ that thus results is an orthogonal and complete set. Hence, it forms an orthogonal representation.

We note here, any L.I. set of N vectors ($N \rightarrow$ dimensions of $\mathcal{H}$) can form a representation. But can orthogonal representation is quite useful to have.

In summary:

1. The basic bras (kets) of an orthogonal representation are simultaneous eigenstates of a complete set of compatible observables.

2. Any set of commuting observables can be made complete by adding certain observables to it.

3. O/N representations are conveniently labeled by the eigenvalues of the compatible observables.

4. Given such a set $\{\langle \lambda_1 \lambda_2 \dots \lambda_K |\}$, any state $|\Psi\rangle$ is completely represented by the numbers $\{\langle \lambda_1 \lambda_2 \dots \lambda_K | \Psi \rangle\}$.

Representation of operators.

As a shorthand let us take the base bras to be $\{\langle\lambda|\}$, $\lambda \doteq \{\lambda^1, \lambda^2, \lambda^3 \ldots \lambda^K\}$.

Consider an operator $\hat{\alpha}$:

$$|v\rangle = \hat{\alpha}|u\rangle \quad \text{— (13)}$$

Using the basis set we get

$$\langle\lambda_i|v\rangle = \sum_{j=1}^{N} \langle\lambda_i|\hat{\alpha}|\lambda_j\rangle\langle\lambda_j|u\rangle \quad \text{— (4)}$$

$$\left(\text{N.B.}\ \sum_{i=1}^{N} \longleftrightarrow \sum_{\lambda_i^1}\sum_{\lambda_i^2}\cdots\sum_{\lambda_i^K} \right)$$

i.e.

$$v_i = \sum_{j=1}^{N} \alpha_{ij}\, u_j \quad \text{— (5)}$$

where the notation is self-explanatory

(5) resembles a matrix equation.

Let us define a column matrix $\overleftrightarrow{V} = \begin{pmatrix} \langle \lambda_1 | V \rangle \\ \langle \lambda_2 | V \rangle \\ \vdots \\ \vdots \end{pmatrix}$

(6) $\left\{ \begin{array}{l} \vec{U} = \begin{pmatrix} \langle \lambda_1 | U \rangle \\ \langle \lambda_2 | U \rangle \\ \vdots \\ \vdots \end{pmatrix} \end{array} \right.$ N entries where N is the dimension of $\mathcal{H}$.

and a square (N×N) matrix $\overleftrightarrow{\alpha}$ s.t.

$$\left(\overleftrightarrow{\alpha}\right)_{ij} = \langle \lambda_i | \hat{\alpha} | \lambda_j \rangle \quad \text{— (7)}$$

wher i, j runs over all possible values the combination of λ's can take.

Then, (5) can be conveniently written as:

$$\boxed{\vec{V} = \overleftrightarrow{\alpha}\,\vec{U}} \quad — (8)$$

Thus, Operators are represented by matrices using an (O/N) representation

States are represented as column (or row if "bra") vectors with entries $V_i \rightarrow i^{th}$ component of V

$$V_i = \langle \lambda_i^1 \lambda_i^2 \cdots \lambda_i^K | V \rangle \quad — (9)$$

Hence, we recover the matrix representation of QM.

Hermitian Matrices: If $\hat{\alpha}$ is Hermitian operator then it is straightforward to show that $\overleftrightarrow{\alpha}$ is a Hermitian matrix satisfying $\overleftrightarrow{\alpha}^{\dagger} = \overleftrightarrow{\alpha}$ — (10)

where $\overleftrightarrow{\alpha}^{\dagger} \equiv \left(\overleftrightarrow{\alpha}^{T}\right)^{*}$ is called the (Hermit.) adjoint of the matrix or the conjugate - transpose.

$$\left(\overleftrightarrow{\alpha}\right)^{T} : \left(\overleftrightarrow{\alpha}^{T}\right)_{ij} = \alpha_{ji} \quad \text{— (11)}$$

$$\left(\overleftrightarrow{\alpha}\right)^{\dagger} : \left(\overleftrightarrow{\alpha}^{\dagger}\right)_{ij} = \alpha_{ji}^{*} \quad \text{— (12)}$$

We can also show that if $\hat{\alpha} \leftrightarrow \overleftrightarrow{\alpha}$ then $\hat{\alpha}^{\dagger} \leftrightarrow \overleftrightarrow{\alpha}^{\dagger}$.

Identity / Unit Operator:

$$\hat{\mathbb{1}} \longleftrightarrow \overleftrightarrow{I} : \left(\overleftrightarrow{I}\right)_{ij} = \delta_{ij} \quad \text{— (13)}$$