Chapter 2: Representation in discrete bases

2-1- Completeness relation and Projection operator

Consider a discrete, complete, and orthonormal basis which is made of countably infinite set of kets $|\chi_1\rangle, |\chi_2\rangle, ..., |\chi_n\rangle$ denote it by $\{|\chi_n\rangle\}$.

The orthonormality condition of the base kets is expressed by

$$\langle \chi_n | \chi_m \rangle = \delta_{nm} \qquad .....(2\text{-}1\text{-}1)$$

where δ_{nm} is the Kronecker delta symbol defined by

$$\delta_{nm} = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases} \qquad .....(2\text{-}1\text{-}2)$$

The completeness relation or closure for this basis is given by:

$$\sum_n |\chi_n\rangle\langle\chi_n| = \hat{I} \qquad .....(2\text{-}1\text{-}3)$$

Where $\hat{I}$ is the identity (unit) operator, when the unit operator acts on any ket, it leaves the ket unchanged.

The projection operator Λ_n is defined as:

$$\Lambda_n = |\chi_n\rangle\langle\chi_n| \qquad .....(2\text{-}1\text{-}4)$$

The completeness relation can be written as

$$\sum_n \Lambda_n = \hat{I} \qquad .....(2\text{-}1\text{-}5)$$

The projection operator has the property:

$$\Lambda_n\Lambda_m = |\chi_n\rangle\langle\chi_n|\chi_m\rangle\langle\chi_m| = \delta_{nm}|\chi_n\rangle\langle\chi_m| = |\chi_n\rangle\langle\chi_n| = \Lambda_n \qquad .....(2\text{-}1\text{-}6)$$

hence

$$\Lambda_n^2 = \Lambda_n \qquad .....(2\text{-}1\text{-}7)$$

The above property is known as idempotency.

2-2- Matrix representation of kets and bras

The completeness property of the basis enables us to expand any state vector $|\psi\rangle$ in terms of the base kets $|\chi_n\rangle$

$$|\psi\rangle = \hat{I}|\psi\rangle = \sum_n |\chi_n\rangle\langle\chi_n|\psi\rangle = \sum_n c_n|\chi_n\rangle \qquad \text{.....(2-2-1)}$$

Where the coefficient $c_n = \langle\chi_n|\psi\rangle$ is the projection of $|\psi\rangle$ on the base vector $|\chi_n\rangle$.

So, within the basis $\{|\chi_n\rangle\}$, the ket $|\psi\rangle$ is represented by the set of its components, c_1, c_2, c_3, … along $|\chi_1\rangle$, $|\chi_2\rangle$, $|\chi_3\rangle$, …, respectively. Hence $|\psi\rangle$ can be represented by a column vector which has a countably infinite number of components:

$$|\psi\rangle = \begin{pmatrix} \langle\chi_1|\psi\rangle \\ \langle\chi_2|\psi\rangle \\ \langle\chi_3|\psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \qquad \text{.....(2-2-2)}$$

Similarly

$$\langle\psi| = \langle\psi|\hat{I} = \sum_n \langle\psi|\chi_n\rangle\langle\chi_n| = \sum_n \langle\chi_n|\psi\rangle^*\langle\chi_n| = \sum_n c_n^*\langle\chi_n| \qquad \text{.....(2-2-3)}$$

Thus, the bra $\langle\psi|$ can be represented by a row vector:

$$\langle\psi| = \begin{pmatrix} \langle\chi_1|\psi\rangle^* & \langle\chi_2|\psi\rangle^* & \langle\chi_3|\psi\rangle^* & \cdots \end{pmatrix} = \begin{pmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{pmatrix} \qquad \text{.....(2-2-4)}$$

The scalar product of two state vectors $|\psi\rangle$ and $|\phi\rangle$ expanded in terms of complete basis set $\{|\chi_n\rangle\}$ is

$$\langle\psi|\phi\rangle = \sum_{nm} c_n^* b_m \langle\chi_n|\chi_m\rangle = \sum_{nm} c_n^* b_m \delta_{nm} = \sum_n c_n^* b_n = \begin{pmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} \qquad \text{.....(2-2-5)}$$

Where the coefficient $b_n = \langle\chi_n|\phi\rangle$ is the projection of $|\phi\rangle$ on the base ket $|\chi_n\rangle$.
Hence a ket is normalized if

$$\langle\psi|\psi\rangle = \sum_n c_n^* c_n \langle\chi_n|\chi_n\rangle = \sum_n c_n^* c_n = \sum_n |c_n|^2 = 1 \quad \text{.....(2-2-6)}$$

Ex. Consider the following two kets: $|\psi\rangle = \begin{pmatrix} -3i \\ 2+i \\ 4 \end{pmatrix}$, $|\phi\rangle = \begin{pmatrix} 2 \\ -i \\ 2-3i \end{pmatrix}$.

a) Find the bra $\langle\phi|$

b) Evaluate the scalar product $\langle\phi|\psi\rangle$.

c) Examine why the products $|\psi\rangle|\phi\rangle$ and $\langle\phi|\langle\psi|$ do not make sense.

Soln:

a) $\langle\phi| = (2 \quad i \quad 2+3i)$

b) $\langle\phi|\psi\rangle = (2 \quad i \quad 2+3i)\begin{pmatrix} -3i \\ 2+i \\ 4 \end{pmatrix} = 7+8i$

c) First, the product $|\psi\rangle|\phi\rangle$ cannot be performed because, from linear algebra, the product of two column matrices cannot be performed. Similarly, since two row matrices cannot be multiplied, the product $\langle\phi|\langle\psi|$ is meaningless.

H.W. Consider the following two kets: $|\psi\rangle = \begin{pmatrix} 5i \\ 2 \\ -i \end{pmatrix}$, $|\phi\rangle = \begin{pmatrix} 3 \\ 8i \\ -9i \end{pmatrix}$.

a) Find $|\psi\rangle^*$ and $\langle\psi|$.

b) Is $|\psi\rangle$ normalized? If not, normalize it.

c) Are $|\psi\rangle$ and $|\phi\rangle$ orthogonal?

2-3- Matrix representation of operators

Consider an operator $\hat{A}$ operates on a ket $|\phi\rangle$ and transforms it into a new ket $|\psi\rangle$, i.e.

$$|\psi\rangle = \hat{A}|\phi\rangle \quad \text{.....(2-3-1)}$$

Using completeness relation

$$\sum_n |\chi_n\rangle\langle\chi_n|\psi\rangle = \hat{A}\sum_m |\chi_m\rangle\langle\chi_m|\phi\rangle$$

$$\sum_n c_n|\chi_n\rangle = \hat{A}\sum_m b_m|\chi_m\rangle \qquad .....(2\text{-}3\text{-}2)$$

Scalar product with $\langle\chi_k|$

$$\sum_n c_n\langle\chi_k|\chi_n\rangle = \sum_m \langle\chi_k|\hat{A}|\chi_m\rangle b_m \qquad .....(2\text{-}3\text{-}3)$$

$$c_n\delta_{kn} = \sum_m A_{km}b_m$$

$$c_k = \sum_m A_{km}b_m \qquad .....(2\text{-}3\text{-}4)$$

Where $A_{km} = \langle\chi_k|\hat{A}|\chi_m\rangle$

Equation (2-3-4) can be written as a set of equations

$$\begin{aligned} c_1 &= A_{11}b_1 + A_{12}b_2 + A_{13}b_3 + \cdots \\ c_2 &= A_{21}b_1 + A_{22}b_2 + A_{23}b_3 + \cdots \\ c_3 &= A_{31}b_1 + A_{32}b_3 + A_{33}b_3 + \cdots \\ &\vdots \end{aligned} \qquad .....(2\text{-}3\text{-}5)$$

Or can be written in matrix form

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} \Leftrightarrow \mathbf{c} = \mathrm{A}\mathbf{b} \qquad .....(2\text{-}3\text{-}6)$$

We see that the operator $\hat{A}$ is represented, within the basis $\{|\chi_n\rangle\}$, by a square matrix A, which has a countably infinite number of columns and a countably infinite number of rows:

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad \text{.....(2-3-7)}$$

In summary, kets are represented by column vectors, bras by row vectors, and operators by square matrices.

2-4- Matrix representation of some other operators

2-4-1- Hermitian adjoint operator

If an operator $\hat{A}$ is represented, within the basis $\{|\chi_n\rangle\}$, by a square matrix A,

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The matrix which represents the operator $\hat{A}^\dagger$ is obtained by taking the complex conjugate of the matrix transpose of A:

$$A^\dagger = A^{\sim *} \quad \text{or} \quad \left(\hat{A}^\dagger\right)_{nm} = \langle\chi_n|\hat{A}^\dagger|\chi_m\rangle = \langle\chi_m|\hat{A}|\chi_n\rangle^* = \left(\hat{A}_{mn}\right)^* = A^*_{mn} \qquad \text{.....(2-4-1)}$$

that is:

$$A^\dagger = \begin{pmatrix} A^*_{11} & A^*_{21} & A^*_{31} & \cdots \\ A^*_{12} & A^*_{22} & A^*_{32} & \cdots \\ A^*_{13} & A^*_{23} & A^*_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad \text{.....(2-4-2)}$$

If an operator $\hat{A}$ is Hermitian, its matrix satisfies this condition:

$$A^\dagger = A \quad \text{or} \quad A^*_{mn} = A_{nm} \qquad \text{.....(2-4-3)}$$

Note that a Hermitian matrix must be square and its diagonal elements real numbers.

2-4-2- Matrix representation of $|\psi\rangle\langle\psi|$

It is easy to see that the product $|\psi\rangle\langle\psi|$ is indeed an operator, since its representation within $\{|\chi_n\rangle\}$ is a square matrix:

$$|\psi\rangle\langle\psi| = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}^{\dagger} = \begin{pmatrix} c_1c_1^* & c_1c_2^* & c_1c_3^* & \cdots \\ c_2c_1^* & c_2c_2^* & c_2c_3^* & \cdots \\ c_3c_1^* & c_3c_2^* & c_3c_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad \text{……(2-4-4)}$$

2-4-3- Trace of an operator

The trace $\mathrm{Tr}(\hat{A})$ of an operator $\hat{A}$ is given within an orthonormal basis $\{|x_i\rangle\}$, by the expression:

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle \chi_n|\hat{A}|\chi_n\rangle = \sum_n A_{nn} \qquad \text{……(2-4-5)}$$

The trace of a matrix is equal to the sum of its diagonal elements.

$$\mathrm{Tr}\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = A_{11} + A_{22} + A_{33} + \cdots \qquad \text{……(2-4-6)}$$

We can ascertain that:

$$\mathrm{Tr}(\hat{A}^{\dagger}) = \left(\mathrm{Tr}(\hat{A})\right)^* \qquad \text{……(2-4-7)}$$

Ex. Show that the trace of a commutator is always zero, i.e. $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.

Soln.

$$\mathrm{Tr}(\hat{A}\hat{B}) = \sum_n \langle \chi_n|\hat{A}\hat{B}|\chi_n\rangle = \sum_n \langle \chi_n|\hat{A}\left(\sum_m |\chi_m\rangle\langle\chi_m|\right)\hat{B}|\chi_n\rangle = \sum_{nm} A_{nm}B_{mn}$$

$$\mathrm{Tr}(\hat{B}\hat{A}) = \sum_m \langle \chi_m|\hat{B}\hat{A}|\chi_m\rangle = \sum_m \langle \chi_m|\hat{B}\left(\sum_n |\chi_n\rangle\langle\chi_n|\right)\hat{A}|\chi_m\rangle = \sum_{mn} B_{mn}A_{nm}$$

$$\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A}) \rightarrow \mathrm{Tr}(\hat{A}\hat{B}) - \mathrm{Tr}(\hat{B}\hat{A}) = 0 \rightarrow \mathrm{Tr}(\hat{A}\hat{B} - \hat{B}\hat{A}) = 0 \rightarrow \mathrm{Tr}\left[\hat{A},\hat{B}\right] = 0$$

2-5- Matrix representation of some quantities

2-5-1- Matrix representation of $\langle\phi|\hat{A}|\psi\rangle$

$$\langle\phi|\hat{A}|\psi\rangle = \langle\phi|\hat{I}\hat{A}\hat{I}|\psi\rangle = \langle\phi|\left(\sum_n |\chi_n\rangle\langle\chi_n|\right)\hat{A}\left(\sum_m |\chi_m\rangle\langle\chi_m|\right)|\psi\rangle$$

$$= \sum_{nm}\langle\phi|\chi_n\rangle\langle\chi_n|\hat{A}|\chi_m\rangle\langle\chi_m|\psi\rangle = \sum_{nm} b_n^* A_{nm} c_m \qquad \text{……(2-5-1)}$$

Hence, the matrix representation of $\langle\phi|\hat{A}|\psi\rangle$ within the basis $\{|\chi_n\rangle\}$ is:

$$\langle\phi|\hat{A}|\psi\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix}^{\dagger} \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \qquad \text{……(2-5-2)}$$

or can be written as:

$$\langle\phi|\hat{A}|\psi\rangle = \begin{pmatrix} b_1^* & b_2^* & b_3^* & \cdots \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \qquad \text{……(2-5-3)}$$

Ex. Consider a matrix A (which represents an operator $\hat{A}$), a ket $|\psi\rangle$ and a bra $\langle\phi|$

$$A = \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix}, \quad |\psi\rangle = \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix}, \quad \langle\phi| = \begin{pmatrix} 6 & -i & 5 \end{pmatrix}$$

a) Calculate the quantities $A|\psi\rangle$, $\langle\phi|A$, $\langle\phi|A|\psi\rangle$ and $|\psi\rangle\langle\phi|$.

b) Find the complex conjugate, the transpose, and Hermitian conjugate of A, $|\psi\rangle$ and $\langle\phi|$.

c) Calculate $\langle\phi|\psi\rangle$ and $\langle\psi|\phi\rangle$.

Soln.

a) $$A|\psi\rangle = \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix} \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = \begin{pmatrix} -5+17i \\ 17+34i \\ 11+14i \end{pmatrix}$$

$$\langle\phi|A = \begin{pmatrix} 6 & -i & 5 \end{pmatrix}\begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix} = \begin{pmatrix} 34-5i & 26+12i & 20+10i \end{pmatrix}$$

$$\langle\phi|A|\psi\rangle = \begin{pmatrix} 6 & -i & 5 \end{pmatrix}\begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix}\begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = 59+155i$$

$$|\psi\rangle\langle\phi| = \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix}\begin{pmatrix} 6 & -i & 5 \end{pmatrix} = \begin{pmatrix} -6+6i & 1+i & -5+5i \\ 18 & -3i & 15 \\ 12+18i & 3-2i & 10+15i \end{pmatrix}$$

b) $A^* = \begin{pmatrix} 5 & 3-2i & -3i \\ i & -3i & 8 \\ 1+i & 1 & 4 \end{pmatrix}$, $\quad |\psi\rangle^* = \begin{pmatrix} -1-i \\ 3 \\ 2-3i \end{pmatrix}$, $\quad \langle\phi|^* = \begin{pmatrix} 6 & i & 5 \end{pmatrix}$

$A^{\sim} = \begin{pmatrix} 5 & -i & 1-i \\ 3+2i & 3i & 1 \\ 3i & 8 & 4 \end{pmatrix}$, $\quad |\psi\rangle^{\sim} = \begin{pmatrix} -1-i & 3 & 2-3i \end{pmatrix}$, $\quad \langle\phi|^{\sim} = \begin{pmatrix} 6 \\ -i \\ 5 \end{pmatrix}$

$A^{\dagger} = \begin{pmatrix} 5 & i & 1+i \\ 3-2i & -3i & 1 \\ -3i & 8 & 4 \end{pmatrix}$, $\quad |\psi\rangle^{\dagger} = \langle\psi| = \begin{pmatrix} -1-i & 3 & 2-3i \end{pmatrix}$, $\quad \langle\phi|^{\dagger} = |\phi\rangle = \begin{pmatrix} 6 \\ i \\ 5 \end{pmatrix}$

c)

$$\langle\phi|\psi\rangle = \begin{pmatrix} 6 & -i & 5 \end{pmatrix}\begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = 4+18i \quad , \quad \langle\psi|\phi\rangle = \begin{pmatrix} -1-i & 3 & 2-3i \end{pmatrix}\begin{pmatrix} 6 \\ i \\ 5 \end{pmatrix} = 4-18i$$

Ex. Write the expectation value of the operator $\hat{A}$ in matrix form with respect to ket state $|\psi\rangle$, if the state $|\psi\rangle$ is represented in terms of complete and orthonormal basis set $\{|\chi_n\rangle\}$.

Soln**.**
The state ket $|\psi\rangle$ is expanded in terms of the basis set $\{|\chi_n\rangle\}$

$$|\psi\rangle = \sum_n |\chi_n\rangle\langle\chi_n|\psi\rangle = \sum_n c_n|\chi_n\rangle$$

We have two cases:

i) If $\{|\chi_n\rangle\}$ are not eigenkets of the operator $\hat{A}$

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{nm} c_n^* \langle\chi_n|\hat{A}|\chi_m\rangle c_m = \sum_{nm} c_n^* A_{nm} c_m$$

$$\langle\hat{A}\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}^{\dagger} \begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & A_{23} & \dots \\ A_{31} & A_{32} & A_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

ii) If $\{|\chi_n\rangle\}$ are eigenkets of the operator $\hat{A}$, i.e. $\hat{A}|\chi_n\rangle = a_n|\chi_n\rangle$

$$\langle\hat{A}\rangle = \sum_{nm} c_n^* \langle\chi_n|\hat{A}|\chi_m\rangle c_m = \sum_{nm} c_n^* a_m \delta_{nm} c_m = \sum_{n} c_n^* a_n I c_n$$

$$\langle\hat{A}\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}^{\dagger} \begin{pmatrix} a_1 & 0 & 0 & \dots \\ 0 & a_2 & 0 & \dots \\ 0 & 0 & a_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

Ex. Formulate in matrix form the raising operator $\hat{a}^+$ for any complete and orthonormal eigen ket $|n\rangle$ of the Hamiltonian of the 1-dimensional Harmonic oscillator.

Soln:

$$\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

Taking scalar product with $\langle m|$

$$\langle m|\hat{a}^+|n\rangle = \sqrt{n+1}\langle m|n+1\rangle$$

$$a^+_{mn} = \sqrt{n+1}\delta_{m,n+1}$$

$$a^+ = \begin{pmatrix} 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

H.W. Formulate in matrix form the lowering operator $\hat{a}^-$ in terms of complete and orthonormal eigen ket $|n\rangle$ of the Hamiltonian of the 1-dimensional Harmonic oscillator.

Ex. Formulate in matrix form the Hamiltonian operator $\hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$ of the 1-dimensional harmonic oscillator, where $|n\rangle$ is any of the complete orthonormal eigen ket.

2-5-2- Matrix representation of the eigenvalue problem

To find the eigenvalues "a" and the eigenvectors $|\psi\rangle$ of an operator $\hat{A}$ satisfy an eigenvalue problem:

$$\hat{A}|\psi\rangle = a|\psi\rangle \qquad \text{……(2-5-4)}$$

one has to work out the matrix representation of this eigenvalue problem.

Inserting unit operator and multiplying by $\langle \chi_m|$, we can cast the eigenvalue equation in the form

$$\langle \chi_m|\hat{A}\hat{I}|\psi\rangle = a\langle \chi_m|\hat{I}|\psi\rangle$$

$$\langle \chi_m|\hat{A}\sum_n |\chi_n\rangle\langle \chi_n|\psi\rangle = a\sum_n \langle \chi_m|\chi_n\rangle\langle \chi_n|\psi\rangle \qquad \text{……(2-5-5)}$$

or

$$\sum_n A_{mn}\langle \chi_n|\psi\rangle = a\sum_n \langle \chi_n|\psi\rangle\delta_{mn} \qquad \text{……(2-5-6)}$$

Which can be rewritten as

$$\sum_n \left(A_{mn} - a\delta_{mn}\right)c_n = 0 \qquad \text{……(2-5-7)}$$

Where $A_{mn} = \langle \chi_m|\hat{A}|\chi_n\rangle$ and $c_n = \langle \chi_n|\psi\rangle$

Equation (2-5-7) represents infinite, homogeneous system of equations for the coefficients $c_n = \langle \chi_n|\psi\rangle$, since the basis $\{|\chi_n\rangle\}$ is made of an infinite number of base kets. This system of equations has trivial solution if $c_n = 0$, and nontrivial solution if the determinant vanishes i.e.

$$\det\left(A_{mn} - a\delta_{mn}\right) = 0 \qquad \text{……(2-5-8)}$$

The problem that arises here is that this determinant corresponds to a matrix with an infinite number of columns and rows. To solve (2-5-8) we need to truncate the basis $\{|\chi_n\rangle\}$ and assume that it contains only N terms, where N must be large enough to guarantee convergence. In this case we can reduce (2-5-8) to the following Nth degree determinant:

$$\begin{vmatrix} A_{11}-a & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22}-a & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33}-a & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN}-a \end{vmatrix} = 0 \qquad \text{……(2-5-9)}$$

Equation (2-5-9) is known as the secular or characteristic equation, which upon solution yield:

- The N eigenvalues (N roots) $a_1, a_2, a_3, ..., a_N$ of A. The set of these N eigenvalues is called the spectrum of A,

$$D = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & a_N \end{pmatrix} \qquad \text{……(2-5-10)}$$

where D is the diagonal matrix collecting all the eigenvalues along the diagonal.

- The N eigenvectors (N column coefficient) $\mathbf{C_1, C_2, C_3, \ldots, C_N}$ of A,

$$\mathbf{C} = (\mathbf{C_1} \quad \mathbf{C_2} \quad \ldots \quad \mathbf{C}_N) = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ c_{N1} & c_{N2} & \cdots & c_{NN} \end{pmatrix} \qquad \text{……(2-5-11)}$$

where each column corresponds to a given eigenvalue,

$$\mathbf{C_1} = \begin{pmatrix} c_{11} \\ c_{21} \\ \vdots \\ c_{N1} \end{pmatrix}, \quad \mathbf{C}_2 = \begin{pmatrix} c_{12} \\ c_{22} \\ \vdots \\ c_{N2} \end{pmatrix}, \ \ldots, \ \mathbf{C}_N = \begin{pmatrix} c_{1N} \\ c_{2N} \\ \vdots \\ c_{NN} \end{pmatrix} \qquad \ldots\ldots(2\text{-}5\text{-}12)$$

- The full eigenvalue problem for a square matrix A is hence given by the single matrix equation:

$$\mathbf{AC} = \mathrm{D}\mathbf{C} \qquad \ldots\ldots(2\text{-}5\text{-}13)$$

where $\mathbf{C}$ is the row matrix of the eigenvectors (a square matrix on the whole), where each column corresponds to a given eigenvalue (the column index).

- Equation (2-5-13) can be written as N eigenvalue equations (one for each eigenvalue),

$$\begin{aligned} \mathrm{A}\mathbf{C_1} &= a_1\mathbf{C_1} \\ \mathrm{A}\mathbf{C}_2 &= a_2\mathbf{C}_2 \\ &\vdots \\ \mathrm{A}\mathbf{C}_N &= a_N\mathbf{C}_N \end{aligned} \qquad \ldots\ldots(2\text{-}5\text{-}14)$$

- If a number of different eigenvectors (two or more) have the same eigenvalue, such eigenvalue is said to be degenerate.

- In the case where the set $\{|\chi_n\rangle\}$ are eigenvectors of the operator $\hat{A}$, then in this basis the matrix representing the operator $\hat{A}$ is diagonal,

$$\mathrm{D} = \mathrm{A} = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & a_N \end{pmatrix} \qquad \ldots\ldots(2\text{-}5\text{-}15)$$

the diagonal elements being the eigenvalues of $\hat{A}$, since

$$\mathrm{A}_{mn} = \langle \chi_m | \hat{A} | \chi_n \rangle = a_n \delta_{mn}$$

Hence, the determination of the eigenvalues of a Hermitian operator is quite equal to diagonalizing its corresponding matrix.

- The trace and determinant of a matrix are given, respectively, by the sum and product of the eigenvalues:

$$\mathrm{Tr}(A) = \sum_n a_n \qquad \text{……(2-5-16)}$$

$$\det(A) = \prod_n a_n \qquad \text{……(2-5-17)}$$

Ex. Find the eigenvalues and the matrix that diagonalize the matrix $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Soln: $\begin{vmatrix} -a & 1 \\ 1 & -a \end{vmatrix} = 0 \rightarrow a^2 = 1 \rightarrow a = \pm 1$

To find the eigenvectors:

i) for $a_1 = -1$

$$A\mathbf{C_1} = a_1\mathbf{C_1} \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_{11} \\ c_{21} \end{pmatrix} = -\begin{pmatrix} c_{11} \\ c_{21} \end{pmatrix} \rightarrow \begin{pmatrix} c_{21} \\ c_{11} \end{pmatrix} = -\begin{pmatrix} c_{11} \\ c_{21} \end{pmatrix} \rightarrow c_{11} = -c_{21}$$

$$\mathbf{C_1} = \begin{pmatrix} c_{11} \\ -c_{11} \end{pmatrix} \rightarrow \mathbf{C}_1^\dagger\mathbf{C_1} = \begin{pmatrix} c_{11} \\ -c_{11} \end{pmatrix}^\dagger \begin{pmatrix} c_{11} \\ -c_{11} \end{pmatrix} = 1 \rightarrow 2|c_{11}|^2 = 1 \rightarrow c_{11} = \frac{1}{\sqrt{2}}$$

$$\mathbf{C_1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

ii) for $a_2 = 1$,

$$A\mathbf{C}_2 = a_2\mathbf{C}_2 \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_{12} \\ c_{22} \end{pmatrix} = \begin{pmatrix} c_{12} \\ c_{22} \end{pmatrix} \rightarrow \begin{pmatrix} c_{22} \\ c_{21} \end{pmatrix} = \begin{pmatrix} c_{21} \\ c_{22} \end{pmatrix} \rightarrow c_{12} = c_{22}$$

$$\mathbf{C}_2 = \begin{pmatrix} c_{12} \\ c_{12} \end{pmatrix} \rightarrow \mathbf{C}_2^\dagger\mathbf{C}_2 = \begin{pmatrix} c_{12} \\ c_{12} \end{pmatrix}^\dagger \begin{pmatrix} c_{12} \\ c_{12} \end{pmatrix} = 1 \rightarrow 2|c_{12}|^2 = 1 \rightarrow c_{12} = \frac{1}{\sqrt{2}} = c_{22}$$

$$\mathbf{C}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The matrix that diagonalize the matrix A is $\mathbf{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ i.e.

$$D = \mathbf{C}^\dagger A\mathbf{C} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Ex. Find the eigenvalues and the normalized eigen vectors for the operator matrix $A = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ and find the unitary matrix that diagonalize it.

Soln:

To find the eigenvalues:

$$\begin{vmatrix} -a & -i & 0 \\ i & -a & 0 \\ 0 & 0 & -a \end{vmatrix} = 0 \rightarrow -a(a^2 - 0) - (-i)(-ia - 0) = 0 \rightarrow a(a^2 - 1) = 0 \rightarrow a = 0, \pm 1$$

To find the eigenvectors:

i) For $a_1 = -1$

$$A\mathbf{C_1} = a_1\mathbf{C_1} \rightarrow \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_{11} \\ c_{21} \\ c_{31} \end{pmatrix} = -\begin{pmatrix} c_{11} \\ c_{21} \\ c_{31} \end{pmatrix} \rightarrow \begin{pmatrix} -ic_{21} \\ ic_{11} \\ 0 \end{pmatrix} = -\begin{pmatrix} c_{11} \\ c_{21} \\ c_{31} \end{pmatrix}$$

$$c_{11} = ic_{21} \ , \quad c_{31} = 0$$

$$\mathbf{C_1} = \begin{pmatrix} ic_{21} \\ c_{21} \\ 0 \end{pmatrix} \rightarrow \mathbf{C_1^\dagger C_1} = \begin{pmatrix} ic_{21} \\ c_{21} \\ 0 \end{pmatrix}^\dagger \begin{pmatrix} ic_{21} \\ c_{21} \\ 0 \end{pmatrix} = 1 \rightarrow 2|c_{21}|^2 = 1 \rightarrow c_{21} = \frac{1}{\sqrt{2}} \rightarrow \mathbf{C_1} = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix}$$

ii) For $a_2 = 0$

$$A\mathbf{C}_2 = a_2\mathbf{C}_2 \rightarrow \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_{12} \\ c_{22} \\ c_{32} \end{pmatrix} = 0 \rightarrow \begin{pmatrix} -ic_{22} \\ ic_{12} \\ 0 \end{pmatrix} = 0 \rightarrow c_{12} = c_{22} = 0 \rightarrow \mathbf{C}_2 = \begin{pmatrix} 0 \\ 0 \\ c_{32} \end{pmatrix}$$

$$\mathbf{C}_2^\dagger\mathbf{C}_2 = \begin{pmatrix} 0 \\ 0 \\ c_{32} \end{pmatrix}^\dagger \begin{pmatrix} 0 \\ 0 \\ c_{32} \end{pmatrix} = 1 \rightarrow |c_{32}|^2 = 1 \rightarrow c_{32} = 1 \rightarrow \mathbf{C}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

iii) For $a_3 = 1$, $A\mathbf{C}_3 = a_3\mathbf{C}_3$

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_{13} \\ c_{23} \\ c_{33} \end{pmatrix} = \begin{pmatrix} c_{13} \\ c_{23} \\ c_{33} \end{pmatrix} \rightarrow \begin{pmatrix} -ic_{23} \\ ic_{13} \\ 0 \end{pmatrix} = \begin{pmatrix} c_{13} \\ c_{23} \\ c_{33} \end{pmatrix} \rightarrow c_{13} = -ic_{23}\ ,\ c_{33} = 0 \rightarrow \mathbf{C}_3 = \begin{pmatrix} -ic_{23} \\ c_{23} \\ 0 \end{pmatrix}$$

$$\mathbf{C}_3^\dagger \mathbf{C}_3 = \begin{pmatrix} -ic_{23} \\ c_{23} \\ 0 \end{pmatrix}^\dagger \begin{pmatrix} -ic_{23} \\ c_{23} \\ 0 \end{pmatrix} = 1 \rightarrow 2|c_{23}|^2 = 1 \rightarrow c_{23} = \frac{1}{\sqrt{2}} \rightarrow \mathbf{C}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix}$$

The matrix that diagonalize the matrix $\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ is $\mathbf{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 0 & -i \\ 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$ i.e.

$$D = \mathbf{C}^\dagger A \mathbf{C} = \frac{1}{2}\begin{pmatrix} i & 0 & -i \\ 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \end{pmatrix}^\dagger \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} i & 0 & -i \\ 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

2-6- Change of bases and Unitary Transformations

2-6-1- Transformations of kets and bras

The transformation from one basis to the other is called a change of basis.
Consider two different complete and orthonormal bases $\{|\chi_n\rangle\}$ and $\{|\chi'_\mu\rangle\}$. Any admissible ket state $|\psi\rangle$ can be expanding in terms of the old basis $|\chi_n\rangle$ as:

$$|\psi_{old}\rangle = \sum_n c_n |\chi_n\rangle \qquad \text{.....(2-6-1)}$$

Where $c_n = \langle x_n|\psi\rangle$ is the components of the ket state $|\psi\rangle$ in terms of the old basis $\{|\chi_n\rangle\}$.

Eq. (2-6-1) can be written in matrix form $\rightarrow$ $|\psi_{old}\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$

The same ket state $|\psi\rangle$ can be represented in the same space but in terms of the new basis set $|\chi'_\mu\rangle$ (in another representation).

$$\left|\psi_{\text{new}}\right\rangle = \sum_{\mu} c'_{\mu}\left|\chi'_{\mu}\right\rangle \qquad .....(2\text{-}6\text{-}2)$$

Where $c'_{\mu} = \left\langle \chi'_{\mu} \middle| \psi \right\rangle$ is the components of the ket state $\left|\psi\right\rangle$ in terms of the new basis $\left|\chi'_{\mu}\right\rangle$

Eq.(2-6-2) can be written in matrix form → $\left|\psi_{\text{new}}\right\rangle = \begin{pmatrix} c'_1 \\ c'_2 \\ c'_3 \\ \vdots \end{pmatrix}$

Transformation from ket state $\left|\psi_{\text{old}}\right\rangle$ to $\left|\psi_{\text{new}}\right\rangle$ (from c_n to c'_{μ}) can be deduced through completeness relation:

$$c'_{\mu} = \left\langle \chi'_{\mu} \middle| \psi \right\rangle = \sum_{n} \left\langle \chi'_{\mu} \middle| \chi_n \right\rangle \left\langle \chi_n \middle| \psi \right\rangle$$

$$c'_{\mu} = \sum_{n} U_{\mu n} c_n \qquad .....(2\text{-}6\text{-}3)$$

Where $U_{\mu n} = \left\langle \chi'_{\mu} \middle| \chi_n \right\rangle$

Equation (2-6-3) can be written in matrix form

$$\begin{pmatrix} c'_1 \\ c'_2 \\ c'_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} & U_{13} & \cdots \\ U_{21} & U_{22} & U_{23} & \cdots \\ U_{31} & U_{32} & U_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \qquad .....(2\text{-}6\text{-}4)$$

Or can be written in compact form

$$\left|\psi_{\text{new}}\right\rangle = \hat{U}\left|\psi_{\text{old}}\right\rangle \quad \rightarrow \quad \mathbf{c}' = U\mathbf{c} \qquad .....(2\text{-}6\text{-}5)$$

The inverse transformation of the above equation (transformation from c'_{μ} to c_n) is:

$$\left|\psi_{\text{old}}\right\rangle = \hat{U}^{\dagger}\left|\psi_{\text{new}}\right\rangle \quad \rightarrow \quad \mathbf{c} = U^{\dagger}\mathbf{c}' \qquad .....(2\text{-}6\text{-}6)$$

Similarly, transformation from basis set $\{\left|\chi_n\right\rangle\}$ to $\{\left|\chi'_{\mu}\right\rangle\}$ can be deduced with the aid of completeness relation:

$$\left|\chi'_{\mu}\right\rangle = \sum_{n} \left|\chi_n\right\rangle \left\langle \chi_n \middle| \chi'_{\mu} \right\rangle \qquad .....(2\text{-}6\text{-}7)$$

$$\left|\chi'_\mu\right\rangle = \sum_n U^\dagger_{n\mu} \left|\chi_n\right\rangle \qquad \text{.....(2-6-8)}$$

Equation (2-6-8) can be written as

$$\left|\chi'_\mu\right\rangle = \hat{U}^\dagger \left|\chi_n\right\rangle \qquad \text{.....(2-6-9)}$$

The inverse transformation of the above equation (transformation from $\left|\chi'_\mu\right\rangle$ to $\left|\chi_n\right\rangle$) is:

$$\left|\chi_n\right\rangle = \hat{U}\left|\chi'_\mu\right\rangle \qquad \text{.....(2-6-10)}$$

One can write

$$\left|\chi_n\right\rangle = \sum_\mu U_{\mu n} \left|\chi'_\mu\right\rangle \qquad \text{.....(2-6-11)}$$

Each basis set $\{\left|\chi_n\right\rangle\}$ and $\{\left|\chi'_\mu\right\rangle\}$ must satisfy the orthonormalization condition:

$\left\langle\chi'_\nu\middle|\chi'_\mu\right\rangle = \delta_{\nu\mu}$ and $\left\langle\chi_m\middle|\chi_n\right\rangle = \delta_{mn}$

Let, first examine the orthonormalization condition $\left\langle\chi'_\nu\middle|\chi'_\mu\right\rangle = \delta_{\nu\mu}$

Starting from eq. (2-6-8) → $\left|\chi'_\mu\right\rangle = \sum_n U^\dagger_{n\mu} \left|\chi_n\right\rangle$

$$\left\langle\chi'_\nu\right| = \sum_m \left\langle\chi_m\right| U_{\nu m} \qquad \text{......(2-6-12)}$$

$$\left\langle\chi'_\nu\middle|\chi'_\mu\right\rangle = \sum_{mn} U_{\nu m} U^\dagger_{n\mu} \left\langle\chi_m\middle|\chi_n\right\rangle = \delta_{\nu\mu} \qquad \text{......(2-6-13)}$$

$$\left\langle\chi'_\nu\middle|\chi'_\mu\right\rangle = \sum_{mn} U_{\nu m} U^\dagger_{n\mu} \delta_{mn} = \delta_{\nu\mu} \qquad \text{......(2-6-14)}$$

$$\left\langle\chi'_\nu\middle|\chi'_\mu\right\rangle = \sum_n U_{\nu n} U^\dagger_{n\mu} = \delta_{\nu\mu} \qquad \text{......(2-6-15)}$$

$$\sum_n U_{\nu n} U^\dagger_{n\mu} = 1 \qquad \text{......(2-6-16)}$$

The above equation can be written in matrix form

$$\hat{U}\hat{U}^\dagger = I \quad \Leftrightarrow \quad \hat{U}^\dagger\hat{U} = I \quad \Leftrightarrow \quad \hat{U}^\dagger = \hat{U}^{-1} \qquad \text{......(2-6-17)}$$

A linear operator whose inverse is its adjoint is called unitary. Due to the above property, the transformation matrix U is called unitary transformation matrix.

H.W. Verify the orthonormalization condition of equation (2-6-11).

2-6-2- Transformations of operators

Let us now examine how operators transform when we change from one basis to another. Let the matrix element of an operator $\hat{A}$ in the old basis $\{|\chi_n\rangle\}$ is:

$$A_{mn} = \langle \chi_m | \hat{A} | \chi_n \rangle \qquad \text{......(2-6-18)}$$

and its matrix element in the new basis is:

$$A'_{\nu\mu} = \langle \chi'_\nu | \hat{A} | \chi'_\mu \rangle \qquad \text{......(2-6-19)}$$

The matrix element $A'_{\nu\mu}$ in the new basis can be expressed in terms of the matrix element in the old basis as follows:

$$A'_{\nu\mu} = \sum_{mn} \langle \chi'_\nu | \chi_m \rangle \langle \chi_m | \hat{A} | \chi_n \rangle \langle \chi_n | \chi'_\mu \rangle$$

$$A'_{\nu\mu} = \sum_{mn} \langle \chi'_\nu | \chi_m \rangle A_{mn} \langle \chi_n | \chi'_\mu \rangle$$

$$A'_{\nu\mu} = \sum_{mn} \langle \chi'_\nu | \chi_m \rangle A_{mn} \langle \chi'_\mu | \chi_n \rangle^*$$

$$A'_{\nu\mu} = \sum_{mn} U_{\nu m} A_{mn} U^\dagger_{n\mu} \qquad \text{.....(2-6-20)}$$

In matrix form:

$$A' = UAU^\dagger \qquad \text{.....(2-6-21)}$$

That is

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger \quad \rightarrow \quad \hat{A}_{new} = \hat{U}\hat{A}_{old}\hat{U}^\dagger \qquad \text{.....(2-6-22)}$$

$$\hat{A} = \hat{U}^\dagger \hat{A}' \hat{U} \quad \rightarrow \quad \hat{A}_{old} = \hat{U}^\dagger \hat{A}_{new} \hat{U} \qquad \text{.....(2-6-23)}$$

H.W. Write the inverse transformation of equation (2-6-21): $A' = UAU^\dagger$