

CHAPTER - 1

SINGLE QUANTUM SYSTEMS

1A. Hilbert Space and other definitions:-

What are quantum states? To define this let us first define What is Hilbert Space?

Def A.1 :- A vector space V is a group of vectors $(|\psi\rangle, |\phi\rangle \in V)$, which can be multiplied by a complex number. So, for a complex number α

$$\alpha |\psi\rangle \in V.$$

Moreover, it is closed under addition

$$|\psi\rangle + |\phi\rangle \in V \quad \forall |\psi\rangle, |\phi\rangle \in V$$

"This will ensure the superposition principle of quantum mechanics which will play an important role in this course. We will discuss it later."

Other properties include that the group must be additive abelian group. The superposition principle is a closure property of that group. Moreover, one must have

$$(i) \quad \alpha (|\psi\rangle + |\phi\rangle) = \alpha |\psi\rangle + \alpha |\phi\rangle$$

$$(ii) \quad (\alpha + \beta) |\psi\rangle = \alpha |\psi\rangle + \beta |\psi\rangle$$

$$(iii) \quad \alpha (\beta |\psi\rangle) = \alpha (\beta |\psi\rangle)$$

$$(iv) \quad 1 |\psi\rangle = |\psi\rangle$$

Additive abelian group:

- (i) $|a\rangle + |b\rangle \in V$ (closure)
 (ii) $(|a\rangle + |b\rangle) + |c\rangle = |a\rangle + (|b\rangle + |c\rangle)$ (Associative)
 $\forall |a\rangle, |b\rangle, |c\rangle \in V$
 (iii) $\exists |0\rangle \in V$ such that (existence of identity)

$$|a\rangle + |0\rangle = |a\rangle \quad \forall |a\rangle \in V$$

- (iv) $\exists -|a\rangle \in V$ such that (existence of inverse)

$$|a\rangle - |a\rangle = 0 \quad \forall |a\rangle \in V$$

For abelian group $|a\rangle + |b\rangle = |b\rangle + |a\rangle$ (Commutativity)
 $\forall |a\rangle, |b\rangle \in V$

Def A2: A Hilbert space is a vector space over the complex numbers 'C', in which there is the notion of "inner product" between the vectors. The inner product between $|\psi\rangle$ & $|\phi\rangle$ is denoted by $\langle \psi | \phi \rangle$.

The properties of inner product are

- (i) $\langle \alpha |\psi\rangle + \beta |\phi\rangle | \chi \rangle = \alpha \langle \psi | \chi \rangle + \beta \langle \phi | \chi \rangle$ (Linearity)
 (ii) $\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^*$ (Skew symmetric)
 (iii) $\langle \psi | \psi \rangle = \|\psi\|^2$ (norm of $|\psi\rangle$)

Properties of norm:

(i) $\|\psi\| \geq 0$ & $\|\psi\| = 0 \Rightarrow |\psi\rangle = 0$

(ii) $\| |\psi\rangle + |\phi\rangle \| \leq \| |\psi\rangle \| + \| |\phi\rangle \|$ (Triangle inequality)

(iii) $\| \alpha |\psi\rangle \| = |\alpha| \| |\psi\rangle \|$; α is complex number.

A Hilbert space must also have a further properties: A sequence of vectors which "tries" to converge, must be able to converge inside the Hilbert space -- This is called completeness.
 Ex: Consider a sequence $\{1/n\}$, in the set $0 < x \leq 1$, the sequence "tries" to converge to 0, but is not able to do so. That set $0 < x \leq 1$ is therefore not complete. is defined in the set of real nos where 0 is not included

* positive real numbers can't form a Hilbert space

Some more definitions:

Def 13:- ORTHOGONALITY: The vectors $|\psi\rangle$ and $|\phi\rangle$ are orthogonal if $\langle \psi | \phi \rangle = 0$. They are non-orthogonal otherwise.

Def 14:- ORTHONORMALITY: A set of states $\{|\psi_i\rangle\}$ is said to be an orthonormal set if $|\psi_i\rangle$ are mutually orthogonal i.e., $\langle \psi_i | \psi_j \rangle = 0$; $i \neq j$ and each state is normalized to unity i.e., $\langle \psi_i | \psi_i \rangle = 1$; $\forall i$.

$$\text{i.e., } \langle \psi_i | \psi_j \rangle = \delta_{ij} \quad \forall i, j \quad (\text{Kronecker delta})$$

Def 15:- ORTHONORMAL BASIS: For any Hilbert space \mathcal{H} , there always exists an orthonormal set of vectors, which are linearly independent, $\{|\psi_i\rangle\}$ in \mathcal{H} so that any element $|\psi\rangle$ can be written as linear combination of the set:

$$|\psi\rangle = \sum_i a_i |\psi_i\rangle \quad ; a_i \text{ being complex numbers.}$$

The set $\{|\psi_i\rangle\}$ is called orthonormal basis of \mathcal{H} . There exists infinitely many basis. Orthonormal basis is also called spanning set of any $|\psi\rangle$.

$$\text{In } \mathbb{C}^2 \quad |\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{or}) \quad |\psi_1\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$|\psi\rangle$ can be written as $a|\psi_1\rangle + b|\psi_2\rangle$ i.e., $|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$

Here

- (i) $a_i = \langle \psi_i | \psi \rangle$
- (ii) $\|\psi\|^2 = \sum_i |a_i|^2$

Def A6: \diamond Number of elements in one the orthonormal basis is defined to be the dimension of a Hilbert space.

"In this whole course, we will mainly deal with finite dimensions"

Def A7:- A Hilbert space is said to be separable if it has countable number of \diamond basis.

1 B. Axioms :-

States of a physical system: Associated to every physical system, there is a separable Hilbert space, whose dimension is equal to the number of degrees of freedom of the physical system.

Why separable? We will be considering systems with finite number of degrees of freedom & hence only finite dimension Hilbert spaces. Such Hilbert spaces are always separable.

Pure states:

Def B1: Suppose that the complete description (about a situation) of a physical system is available. Then this situation is associated with a vector $|\psi\rangle$ of the corresponding Hilbert space \mathcal{H} . Such a situation or vector is called a pure state.

Ex: \rightarrow Spin up and spin down - two degrees of freedom. So this physical system is described by the 2-dim Hilbert space.

$$\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$$

forms an orthonormal basis. Any other state can be written as convex combination of

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}} [|\uparrow_z\rangle + i|\downarrow_z\rangle]$$

\exists other orthonormal basis $\{|1_x\rangle, |1_x\rangle\}$, $\{|1_y\rangle, |1_y\rangle\}$

* The inner product of $|1_y\rangle$ and $|1_z\rangle$:

$$\begin{aligned} & \langle 1_y | 1_z \rangle \\ &= \frac{1}{\sqrt{2}} \left(\langle 1_z | + i \langle 1_z | \right) | 1_z \rangle \\ &= \frac{1}{\sqrt{2}} \end{aligned}$$

* Suppose spin of an electron is proportional polarized in the up-z-direction, then we describe it by $|1_z\rangle$, a pure state. If it is polarized in up x-direction we describe up by $|1_x\rangle$ which can be written as $\frac{1}{\sqrt{2}}(|1_z\rangle + |1_z\rangle)$. This is another pure state.

Def B2:- QUBIT - A qubit is a state in a 2-dimensional Hilbert space. The indivisible unit of classical information is the bit which takes one of the 2 possible values $\{0, 1\}$. The corresponding unit of quantum information is called "quantum bit" or "qubit". It describes a state in the simplest possible quantum system.

A smallest nontrivial Hilbert space in 2-dimensional orthonormal basis for a 2d Hilbert space denoted as \mathcal{H}^2 as $\{|0\rangle, |1\rangle\}$. The most general state is

$$\alpha|0\rangle + \beta|1\rangle$$

where α, β are complex numbers and $|\alpha|^2 + |\beta|^2 = 1$.

Def B3:- Adjoints - A is any linear operator on Hilbert space \mathcal{H} . \exists a unique linear operator A^\dagger on V such that $\forall |v\rangle, |w\rangle \in \mathcal{H}$

$$(|v\rangle, A|w\rangle) = (A^\dagger|v\rangle, |w\rangle)$$

This linear operator is called adjoint or Hermitian conjugate of A .

Def B4: Self adjoint: An operator A whose adjoint is A is called Hermitian or self adjoint operator.

An important class of Hermitian operators is the projectors.

Def B5: A projector P on a Hilbert space H is a linear Hermitian operator on H , such that

$$P^2 = P \quad (P^\dagger = P)$$

Any projector can always be written as

$$P = \sum_i |\psi_i\rangle\langle\psi_i|$$

where $\{|\psi_i\rangle\}$ are orthonormal set of H . If a projector can be written as $|\psi\rangle\langle\psi|$, it is said to be rank one.

$$\star \rightarrow \text{If } P = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

$$P^2 = \sum_{ij} \lambda_i \lambda_j |\psi_i\rangle\langle\psi_i| \langle\psi_i|\psi_j\rangle |\psi_j\rangle\langle\psi_j|$$

$$= \sum_i \lambda_i^2 |\psi_i\rangle\langle\psi_i| \quad \because \lambda_i^2 = \lambda_i \Rightarrow \lambda_i = 0, 1$$

(Rank 2)?

Theorem A.1: Spectral theorem for Hermitian operators
Any Hermitian operator S on a Hilbert space H can be written in its special decomposition as

$$S = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

where $|\psi_i\rangle \in H$ are orthonormal vectors and λ_i are real numbers. λ_i and $|\psi_i\rangle$ are eigenvalues and eigenvectors of S .

Identity: E.g. For any orthonormal basis $\{|\psi_i\rangle\}$ of a Hilbert space \mathcal{H} , one has

$$\sum_i |\psi_i\rangle\langle\psi_i| = I$$

where I is the identity operator of \mathcal{H} in \mathbb{C}^2

$$\left[|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z| \right] = I$$

Def B.6: Positive operators: A linear operator P on \mathcal{H} is said to be positive if

$$\langle\psi|P|\psi\rangle \geq 0 \quad \forall |\psi\rangle \in \mathcal{H}.$$

It is enough to check that $\langle\psi_i|P|\psi_i\rangle \geq 0$ for some orthonormal basis $\{|\psi_i\rangle\}$ of \mathcal{H} . Any operator projector is a positive operator.

Def B.7: Trace: The trace of a linear operator P on \mathcal{H} is defined as

$$\sum \langle\psi_i|P|\psi_i\rangle$$

for any orthonormal basis $\{|\psi_i\rangle\}$ in \mathcal{H} .

NOTE: It is independent of the chosen basis.

Mathematical Properties of a pure state

- i) A pure state is self adjoint
- ii) It is positive, i.e., all eigenvalues are positive.
- iii) $\text{tr}(P) = 1$, unit trace.
- iv) Additionally $\text{tr}(P^2) = \text{tr}(P) = 1$.

Mixed States

Suppose now that we are not sure about the exact physical situation of the system. But, we know that the system is in the pure state $|\psi_i\rangle$ with probability p_i , then the state of the system is described by the following linear operator on \mathcal{H} :

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| ; p_i \geq 0 \text{ and } \sum_i p_i = 1.$$

NOTE: The $|\psi_i\rangle$ may be non-orthogonal

(i) ρ is Hermitian: $\rho = \rho^\dagger = (\rho^*)^T$

(ii) ρ is positive: let $|\phi\rangle$ be an arbitrary vector in state space

$$\begin{aligned} \langle\phi|\rho|\phi\rangle &= \sum_i p_i \langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle \\ &= \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0 \end{aligned}$$

(iii) ρ is of unit trace: $\text{tr } \rho = \sum_i p_i \text{tr } (|\psi_i\rangle\langle\psi_i|)$

$$= \sum_i p_i = 1$$

ex: $\rho = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix}$ is positive matrix

$\rho^\dagger = \begin{pmatrix} 1 & 0 \\ 1 & 2 \end{pmatrix} \neq \rho$ is not Hermitian

$\therefore \rho$ is a positive matrix which is not Hermitian.

Corollary of spectral theorem:

If ρ is hermitian, positive and of unit trace, then spectral theorem guarantees that

$$\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$$

where p_i are probabilities and $\{|\phi_i\rangle\}$ are orthonormal basis.

Def B.8: A mixed state on \mathcal{H} is defined as a hermitian, positive and unit trace operator on \mathcal{H} . It is said to be pure if it can be written as $|\phi\rangle\langle\phi|$, i.e., only one eigenvalue is non zero. In that case, we write it as either $|\phi\rangle$ or $|\phi\rangle\langle\phi|$.

Proposition B.1: A state ρ is pure if and only if

$$\rho^2 = \rho \quad \text{or} \quad \text{Tr}(\rho^2) = 1$$

\Rightarrow By using spectral theorem, $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$

$$\text{Tr}(\rho^2) = \sum_i p_i^2 \quad p_i^2 \leq p_i$$

$$\sum_i p_i^2 \leq \sum_i p_i = 1$$

equality holds iff $p_i^2 = p_i \forall i$. If ρ is pure state then $\sum_i p_i^2 = \sum_i p_i = 1$.