CH # 2

Mathematical Tools of Quantum Mechanics:

Dynamical quantities like position, momentum kinetic energy, potential energ etc, which form the objectives of measurent in experimental Physics are called observables. In quantum mechanics, each observable is represented by an operator which acts on the wavefunction $\psi(\underline{x},t)$ ~~to produce a new function~~. Before going into details of quantum mechanics, we first develop the mathematical theory of operators which would be needed for later understanding of the subject

1-a Hilbert Space:

A Hilbert space consists of a se
of vector space $\psi, \phi, \chi, \ldots$ and
a set of scalar space $a, b, c, \ldots$
In the Schroedinger equation, the
solution $\psi(\underline{x}, t)$ may be multip
by a constant and it
still remains a solution.

Thus the equation

$$\int_{-\infty}^{\infty} \rho(\underline{x}, t)\, d\underline{x} = 1$$

restricts the wavefunction $\psi(\underline{x}, t)$
to a class of functions for which

$$\int_{-\infty}^{\infty} |\psi(\underline{x}, t)|^2\, d\underline{x} < \infty$$

Such functions are known as square
integrable functions.

A set $L^2(\mathbb{R}^3)$ of all square integrable
space
functions form a vector space over three dimensions Euclidean space $\mathbb{R}^3$.

Euclidean space consists of the two dimensional Euclidean plane. It is modelled by the real coordinate space $(\mathbb{R}^n)$ of the same dimension. In one dimension, this is the real line, in 2D, it is the Cartesian plane, and in higher dimension it is a coordinate space.

The inner product or scalar product is defined as:

for $\phi, \psi \in L^2(\mathbb{R}^3)$, the inner or scalar product of ϕ and ψ is.

$$(\phi, \psi) = \int_{-\infty}^{\infty} \phi^*(\underline{x}, t)\, \psi(\underline{x}, t)\, d\underline{x}$$

which satisfies

i) $(\phi, \phi) \geq 0$

ii) $(\phi, \phi) = 0 \iff \phi = 0$

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iii) $(a\phi, \psi) = a^*(\phi, \psi)$

iv) $(\phi, a\psi + b\chi) = a(\phi, \psi) + b(\phi, \chi)$

v) $(\phi, \psi) = (\psi, \phi)^*$

The space L^2 together with the in[ner]
Product defined above form a Hilb[ert]
space $\mathcal{H} = L^2(\mathbb{R}^3)$.

Orthogonality:

Two functions $\phi, \psi \in L^2(\mathbb{R}^3)$ a[re]
Said to be orthogonal to each oth[er]
if

$$\int_{-\infty}^{\infty} \phi^*(\underline{x}, t)\,\psi(\underline{x}, t)\,d\underline{x} = \int_{-\infty}^{\infty} \psi^*(\underline{x}, t)\,\phi(\underline{x}, t)$$

or
$$(\phi, \psi) = (\psi, \phi) = 0$$

Normalization:

$$\int_{-\infty}^{\infty} \phi^* \phi \, dx = \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

Linearly Independent Functions:

Two functions $\phi, \psi \in L^2$ are said to be linearly independent if

$$a\phi + b\psi = 0 \implies a, b = 0.$$

Let us ~~write~~ start with

$$a\phi + b\psi = 0 \quad \text{—— (1)}$$

Multiplying both sides by ϕ^* and integrating

$$a\int_{-\infty}^{\infty} \phi^*\phi \, d\underline{x} + b\int_{-\infty}^{\infty} \phi^*\psi \, d\underline{x} = 0$$

$$\Rightarrow a + b\int_{-\infty}^{\infty} \phi^*\psi \, d\underline{x} = 0$$

If ϕ and ψ are orthogonal, then

$$a = 0$$

The equation (1) implies that

$$b = 0.$$

We conclude when ψ and ϕ are orthogonal to each other, they are linearly independent.

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Odd and Even Functions :

If for $\psi(\underline{x},t) \in L^2(\mathbb{R}^3)$, then

$$\psi(-\underline{x},t) = \psi(\underline{x},t)$$

$\psi(\underline{x},t)$ is said to be even or even parity function.

If

$$\psi(-\underline{x},t) = -\psi(\underline{x},t)$$

$\psi(\underline{x},t)$ is said to be odd or odd parity function.

Orthonormal Set of Functions :

Let $\phi_1, \phi_2, \ldots, \phi_n \in L^2(\mathbb{R}^3)$, then the orthogonality condition for these functions is

$$\int_{-\infty}^{\infty} \phi_m^* \phi_n \, d\underline{x} = (\phi_m, \phi_n) = 0$$

$\forall\ m \neq n$

The functions are normalized if

$$\int_{-\infty}^{\infty} \phi_n^* \phi_n \, d\underline{x} = (\phi_n, \phi_n) = 1$$

If both orthogonality and normalization conditions are satisfied then the set $\{\phi_n\}$ is said to be orthonormal set.

So for the orthonormal functions

$$\int_{-\infty}^{\infty} \phi_m^*(x,t)\,\phi_n(x,t)\,dx = \delta_{mn}$$

where δ_{mn} is the ~~Kr~~ Kronecker delta defined by.

$$\delta_{mn} = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

Complete Orthonormal Set:

The functions $\phi_1, \phi_2, \ldots, \phi_n \in L^2(\mathbb{R}^3)$ from a complete orthonormal set, if any function $\psi \in L^2(\mathbb{R}^3)$ can be expanded in terms of them i.e.

$$\psi = \sum_n a_n \phi_n$$

4-a It follows that

$$\int \phi_m^* \psi \, d\underline{x} = (\phi_m, \psi)$$

$$= \sum_n a_n (\phi_m, \phi_n)$$

$$= \sum_n a_n \delta_{mn}$$

maximum possible number of linearly independent vectors belonging to that space

$$\boxed{\int \phi_m^* \psi \, d\underline{x} = a_m},$$

The complete orthonormal set $\{\phi_n\}$ (called basis), $n = 1, 2, 3, \ldots$, $\phi_1 \in L^2$, $\phi_2 \in L^2$ $\phi_n \in L^2$ constitutes a basis if every (vectors) function $\psi \in L^2$ can be expressed as a linear combination of basis functions

$$\psi = \sum_n a_n \phi_n.$$

The co-efficients a_n are determi[ned] as.

$$a_n = (\phi_n, \psi) = \int \phi_n^* \psi \, dx$$

(5)

The set of numbers a_n are said to represent or of ψ in the $\{\phi_n\}$ basis.

Let ϕ and ψ be two wavefunction which can be expanded as

$$\phi = \sum_n a_n \phi_n$$

$$\psi = \sum_m b_m \phi_m$$

Their scalar product is

$$(\phi, \psi) = \left(\sum_n a_n \phi_n , \sum_m b_m \phi_m \right)$$

$$= \sum_{n,m} a_n^* b_m (\phi_n \cdot \phi_m)$$

$$= \sum_{n,m} a_n^* b_m \, \delta_{nm}$$

If $n = m$

$$= \sum_n a_n^* b_n$$

In particular

$$(\psi, \psi) = \sum_n |b_n|^2$$

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CAUCHY-SCHWARZ INEQUALITY

It is useful in many different setting such as linear Algebra, vector Algebra, Probability Theory and analysis and also other areas.

For any two functions $\varphi, \psi \in L^2$

$$(\varphi,\varphi)(\psi,\psi) \geq |(\varphi,\psi)|^2$$

or. equivalently

$$\|\varphi\| \|\psi\| \geq |(\varphi,\psi)|$$

Double modulus is reserved for the norm of the vector and single is usually for the absolute value also called magnitude of complex number.

where

$$\|\varphi\| = \sqrt{(\varphi,\varphi)}, \quad \|\psi\| = \sqrt{(\psi,\psi)}$$

√ magnitude of real number

Proof.

For any $\lambda \in \mathbb{C}$ (set of Complex numbers) and $\varphi, \psi \in L^2(\mathbb{R}^3)$, we have

$$0 \leq (\varphi+\lambda\psi, \varphi+\lambda\psi)$$

$$= (\varphi,\varphi) + \lambda^*(\psi,\varphi) + \lambda(\varphi,\psi) + \lambda\lambda^*(\psi,\psi).$$

write

$$a = (\varphi, \varphi)$$

$$b = (\psi, \varphi)$$

$$c = (\psi, \psi)$$

So we have,

$$a + \lambda^* b + \lambda b^* + \lambda\lambda^* c \geq 0$$

suppose that $c \neq 0$, so that $\psi \neq 0$

Now choose

$$\lambda = -b/c.$$

Then we have

$$a - \frac{bb^*}{c} - \frac{bb^*}{c} + \frac{bb^*}{c} \geq 0$$

or

$$a - \frac{bb^*}{c} \geq 0$$

$$ac - |b|^2 \geq 0$$

$$ac \geq |b|^2$$

i.e.

$$\boxed{(\varphi, \varphi)(\psi, \psi) \geq |(\varphi, \psi)|^2}$$

Hence proved.

6-9 Operators → function over a space of fn's

"An operator $\hat{A}$ is a transformation which takes any function in a ~~space~~ function space of to another function in the same space."

If $\psi \in L^2(\mathbb{R}^3)$, then $\hat{A}\psi \in L^2(\mathbb{R}^3)$

$$\hat{A} : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}^3)$$

The simplest example of an operator is

$$\hat{A}(x) = x$$

$\hat{A}(x) = x$ acting on $\psi \in L^2(\mathbb{R})$

$$\hat{A}\psi = x\,\psi$$

Another example is a differential operator

$$\hat{A}\left(\frac{\partial}{\partial x}\right)$$

e.g.

$$\frac{\partial^2}{\partial x^2},\quad x\frac{\partial}{\partial x},\quad \frac{\partial^2}{\partial x^2} - x^2$$

The most general operator we meet is a function of x and $\frac{\partial}{\partial x}$

$$\hat{A} = \hat{A}\left(x, \frac{\partial}{\partial x}\right)$$

Operator Equation:

In order to get an idea of an operator equation, let us consider an operator

$$\hat{A}(x, \frac{\partial}{\partial x}) = \frac{\partial}{\partial x} x$$

we need to know that som ~~sum~~ of

i) Sum of two operators gives another operator:

$$\hat{C} = \hat{A} + \hat{B} : \quad \hat{C}\psi = (\hat{A} + \hat{B})\psi$$
$$= \hat{A}\psi + \hat{B}\psi$$

ii) Product of operators:

$$\hat{D} = \hat{A}\hat{B} : \quad \hat{D}\psi = (\hat{A}\hat{B})\psi = \hat{A}(\hat{B}\psi)$$

It is important to know that $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ may not be equal. i.e.

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

For example if

$$\hat{A} = \frac{\partial}{\partial x}$$
$$\hat{B} = x$$

Then

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$$\hat{A}\hat{B}\psi = \left(\frac{\partial}{\partial x}x\right)\psi = \frac{\partial}{\partial x}(x\psi)$$

$$= \left(1 + x\frac{\partial}{\partial x}\right)\psi$$

$$\hat{B}\hat{A}\psi = x\frac{\partial}{\partial x}\psi$$

So

$$\boxed{\hat{A}\hat{B}\psi = \left(1 + \hat{B}\hat{A}\right)\psi}$$

The above equation is true for every function ψ, therefore, the resulting operator is.

$$\boxed{\hat{A}\hat{B} = 1 + \hat{B}\hat{A}}$$

Two special operators are

* Null (zero) operator: $\hat{O}$

$$\hat{O}\psi = 0, \quad \hat{A}\hat{O} = \hat{O}\hat{A} = \hat{O}$$

* Unit operator: $\hat{1}$

$$\hat{1}\psi = \psi, \quad \hat{1}\hat{A} = \hat{A}\hat{1} =$$

The square of an operator is defined as

$$\hat{A}^2 = \hat{A}\hat{A}$$

$$\hat{A}^2\psi = \hat{A}(\hat{A}\psi)$$

Similarly

$$\hat{A}^n = \hat{A}\hat{A}^{n-1} = \hat{A}\hat{A}\hat{A}^{n-2} = \underbrace{\hat{A}\hat{A}\cdots\hat{A}}_{n\text{-factors}}$$

If two operators $\hat{A}$ and $\hat{B}$ are related by $\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{1}$

then they are said to be reciprocal to each other and $\hat{B}$ is called the inverse of $\hat{A}$ denoted by $\hat{A}^{-1}$.

An operator for which an in inverse exists is said to be non-singular, where as one for which no inverse exists is signular.

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Commutator:

Let $\hat{A}$ and $\hat{B}$ are two operators, then Commutator is defined by

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

In general

$$[\hat{A}, \hat{B}] \neq 0$$

example:

$$\left[x, \frac{\partial}{\partial x}\right] \psi(x) = \left(x \frac{\partial}{\partial x} - \frac{\partial}{\partial x} x\right) \psi(x)$$

$$= x \frac{\partial}{\partial x} \psi - \frac{\partial}{\partial x}(x\psi)$$

$$= x \frac{\partial}{\partial x} \psi - \psi - x \frac{\partial}{\partial x} \psi$$

$$= \left(x \frac{\partial}{\partial x} - 1 - x \frac{\partial}{\partial x}\right) \psi$$

$$= -1 \, \psi(x)$$

Since this is true for any ψ, therefore

$$\boxed{\left[x, \frac{\partial}{\partial x}\right] = -1}$$

Adjoint operator:

An operator $\hat{A}^{+}$ is called the adjoint operator to $\hat{A}^{*}$ if

$$\int \hat{A}^{+} \phi^{*} \psi \, dx = \int \phi^{*} \hat{A}^{+} \psi \, dx$$

or

$$(A\phi, \psi) = (\phi, \hat{A}^{+}\psi)$$

Hermitian operator:

An operator $\hat{A}$ is said to be Hermitian or self-adjoint if

$$\hat{A} = \hat{A}^{+}$$

In this case

$$(\hat{A}\phi, \psi) = (\phi, \hat{A}\psi)$$

or

$$\int \hat{A}^{+} \phi^{*} \psi \, dx = \int \phi^{*} \hat{A} \psi \, dx$$

Theorem:

For any two operators $\hat{A}$ and $\hat{B}$

$$(\hat{A}\hat{B})^{+} = \hat{B}^{+} \hat{A}^{+}$$

9.a <u>Proof</u>: By definition

$$\int (\hat{A}\hat{B})^{*} \varphi^{*} \psi \, dx = \int \varphi^{*} (\hat{A}\hat{B})^{t} \psi \, dx$$

L.HS gives

$$\int (\hat{A}\hat{B})^{*} \varphi^{*} \psi \, dx = \int \hat{A}^{*} \hat{B}^{*} \varphi^{*} \psi \, dx$$

$$= \int (\hat{B}^{*} \varphi^{*}) \hat{A}^{t} \psi \, dx$$

$$= \int \varphi^{*} \hat{B}^{t} \hat{A}^{t} \psi \, dx$$

So we have

$$\int \varphi^{*} \hat{B}^{t} \hat{A}^{t} \psi \, dx = \int \varphi^{*} (\hat{A}\hat{B})^{t} \psi \, dx$$

since this holds for any φ, ψ then

$$\boxed{(\hat{A}\hat{B})^{t} = \hat{B}^{t} \hat{A}^{t}}$$

<u>Theorem</u>:

$$(\hat{A}^{*})^{t} = (\hat{A}^{t})^{*}$$

<u>Proof</u>: By definition:

$$\int \hat{A}^{*} \varphi^{*} \psi \, dx = \int \varphi^{*} \hat{A}^{t} \psi \, dx$$

Taking complex conjugate on both sides

$$\int (\hat{A}^{*})^{*} (\phi^{*})^{*} \psi^{*} dx = \int (\phi)^{*} (\hat{A}^{+})^{*} \psi^{*} dx$$

$$\int (\phi^{*})^{*} (\hat{A}^{*})^{+} \psi^{*} dx = \int \phi (\hat{A}^{+})^{*} \psi^{*} dx$$

$$\int \phi (\hat{A}^{*})^{+} \psi^{*} dx = \int \phi (\hat{A}^{+})^{*} \psi^{*} dx$$

Since this is hold for any ψ and ϕ,

therefore $$(\hat{A}^{*})^{+} = (\hat{A}^{+})^{*}$$

<u>Unitary Operator:</u>

An operator U is said to be unitary if it has an inverse U^{-1} and an adjoint U^{+} such that

$$U^{-1} = U^{+}$$

$$UU^{+} = U^{+}U = 1$$

The action of U on function $\psi(x,t)$ preserves the norm

$$(U\phi, U\psi) = (\psi, U^{+}U\psi) = (\phi, \psi)$$

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Projection Operator:

An operator P is said to be a projection operator if it is Hermitian

$$P^{\dagger} = P$$

and idempotent

$$P^2 = P.$$

Function of an opertor:

Any function $f(x)$ can be ex[illegible] as a power series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n.$$

The corresponding function of the operator $\hat{A}$ is ~~the operator~~ $f(A)$ defi[illegible] by.

$$f(A) = \sum_{n=0}^{\infty} a_n A^n.$$

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