Eigenvalues and Eigenfunctions of an operator:

In general, when an operator $\hat{A}$ operates upon a function, a different function is obtained,

$$\hat{A}\psi = \phi$$

But there may be some function ψ with the property

$$\hat{A}\psi = \lambda\psi \quad \text{——} (*)$$

where λ is a scalar. In this case the action of $\hat{A}$ on ψ yields the same the function ψ multiplied by a scaler λ. The function ψ is then called an eigenfn of the operator $\hat{A}$ belonging to the eigenvalue λ. The equation $(*)$ is referred to as the eigenvalue equation. Examples are

$$\frac{d}{dx}\left(e^{\alpha x}\right) = \alpha\left(e^{\alpha x}\right)$$

$$\frac{d^2}{dx^2}\sin 4x = -16\sin 4x.$$

11-a

Degenerate Eigenvalues:

In general, an operator can have several eigenvalues and eigenfunctions

$$\hat{A}\psi_n = \lambda_n \psi_n$$

The set $\{\lambda_n\}$ of all the eigenvalue[s of] $\hat{A}$ is called the spectrum of the oper[ator]. When an operator acts on several lin[early] independent functions and give the [same] eigenvalue λ, then λ is called a deg[enerate] eigenvalue and the number of linea[rly] independent eigenfunctions is calle[d] the degree of ~~degenerate~~ degenera[cy].

Example:

$$\frac{d^2}{dx^2}\cos ax = -a^2 \cos ax, \quad \frac{d^2}{dx^2}\sin ax = -a^2 [\sin ax]$$

Simultaneous Eigenfunctions:

Let $\hat{A}$ and $\hat{B}$ be two operators. An eigenfunction ψ is said to be a simultaneous eigenfunction of $\hat{A}$ and $\hat{B}$ if

$$\hat{A}\psi = \lambda\psi$$
$$\hat{B}\psi = \mu\psi$$

If there exists a complete set of simultaneous eigenfunctions of two linearly operators, then the operators are said to be compatible. The operators which are not compatible are known as incompatible operators.

Theorem: If two operators are compatible, then they commute with each other.

Proof: Let $\hat{A}$ and $\hat{B}$ be two compatible operators:

$$\hat{A}\psi = \lambda\psi$$
$$\hat{B}\psi = \mu\psi$$

12-9

Now

$$\hat{A}\hat{B}\psi = \hat{A}\mu\psi = \mu\hat{A}\psi = \mu\lambda\psi$$

$$\hat{B}\hat{A}\psi = B\lambda\psi = \lambda\hat{B}\psi = \mu\lambda\psi$$

$$\Rightarrow \quad (\hat{A}\hat{B} - \hat{B}\hat{A})\psi = 0$$

Since this is true for all eigenfun
therefor

$$(\hat{A}\hat{B} - \hat{B}\hat{A}) = 0, \quad \psi \neq 0$$

$$\Rightarrow \quad [\hat{A}, \hat{B}] = 0$$

Hence compatible operators comm
with each other.

<u>Theorem:</u> The eigenvalues of a Herm
operator are real.

<u>Proof:</u> Let $\hat{A}$ be a Hermitian ope

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

Let ψ be an eigenfunction of $\hat{A}$,
then

$$\hat{A}\psi = \lambda\psi \quad \text{---(1)}$$

Multiplying by ψ^* from left side and integrating over the whole space

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

$$= \lambda \quad \text{---} (2)$$

Now take complex conjugate of equ (1)

$$\hat{A}^* \psi^* = \lambda^* \psi^*$$

Multiplying by ψ from right side and integrating over the whole space

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

$$\int \psi^* \hat{A}^\dagger \psi \, dx = \lambda^* \int \psi^* \psi \, dx$$

Since $\hat{A}$ is Hermitian, $\hat{A}^\dagger = A$, we may write

$$\int \psi^* \hat{A} \psi \, dx = \lambda^* \quad \text{---} (3)$$

Comparing equation (2) and (3),

$$\Rightarrow \lambda = \lambda^*$$

Hence, eigenvalues of corresponding a Hermitian operator are real.

Theorem: The total probability dens of a wavefunction is constant if only if the Hamiltonian of the system is Hermitian.

Proof: Let the total probability be c

i.e.

$$\frac{d}{dt}\left(\int \psi^* \psi \, dx\right) = 0$$

or.

$$\int \left(\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right) dx = 0 \quad \text{--- (1)}$$

The Schrodinger equation gives

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$\frac{\partial \psi}{\partial t} = -i \left(\frac{\hat{H}}{\hbar} \right) \psi$$

By taking the complex conjugate of the Schrodinger equation, we get

$$\frac{\partial \psi^*}{\partial t} = i\left(\frac{\hat{H}^*}{\hbar}\right)\psi^*$$

Now the equation (1) can be expressed as

$$\frac{i}{\hbar}\int \hat{H}^*\psi^*\psi\, dx - \frac{i}{\hbar}\int \psi^*\hat{H}\psi\, dx = 0$$

$\Rightarrow$

$$\frac{i}{\hbar}\int \psi^*\hat{H}^\dagger\psi\, dx - \frac{i}{\hbar}\int \psi^*\hat{H}\psi\, dx = 0$$

Since this is true for any ψ, therefore

$$\boxed{\hat{H}^\dagger = \hat{H}}$$

i.e. for total probability to be constant, the Hamiltonian operator is Hermitian.

<u>Converse:</u>

Let the Hamiltonian be Hermitian.

$$\hat{H}^\dagger = \hat{H}$$

i.e

$$\int \hat{H}^*\psi^*\psi\, dx = \int \psi^*\hat{H}\psi\, dx \quad (1)$$

14-a The Schrodinger equation is

$$\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Complex conjugation gives

$$\hat{H}^* \psi^* = -i\hbar \frac{\partial \psi^*}{\partial t}$$

Equ: ① now can be written as

$$-i\hbar \int \frac{\partial \psi^*}{\partial t} \psi \, dx = i\hbar \int \psi^* \frac{\partial \psi}{\partial t} \, dx$$

$$\Rightarrow i\hbar \left(\int \left(\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right) dx \right) = 0$$

$$\Rightarrow \frac{d}{dt} \left(\int \psi^* \psi \, dx \right) = 0.$$

Hence, the total probability is constant

Theorem: The product of two commuti Hermitian operators is Hermitian.

Proof: Let $\hat{A}$ and $\hat{B}$ be two commuti Hermitian operators, then

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

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

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

$\because \hat{B}^+ = \hat{B}$

$$= \int \phi^* \hat{A} \hat{B} \psi \, dx$$ $\because [\hat{A}, \hat{B}] = 0$

$\hat{A}\hat{B} = \hat{B}\hat{A}$

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

Hence $(\hat{A}\hat{B})$ is Hermitian.

Theorem: The eigenfunctions of a Hermitian operator corresponding to different eigenvalues are mutually orthogonal.

Proof: Let λ_m and λ_n be two different sets of eigenvalue for Hermitian operator $\hat{A}$

i.e.

$$\hat{A} \psi_m = \lambda_m \psi_m \quad \text{—— (1)}$$

$$\hat{A} \psi_n = \lambda_n \psi_n \quad \text{—— (2)}$$

By difinition

$$\int \hat{A}^* \psi_m^* \psi_n \, dx = \int \psi_m^* \hat{A} \psi_n \, dx$$

15 - a

Taking complex conjuate on both s

$$\int \hat{A}\psi_m \psi_n^{*} dx = \int \psi_m (\hat{A}\psi_n)^{*} dx$$

Now making use of (1) and (2)

$$\lambda_m \int \psi_m \psi_n^{*} dx = \lambda_n^{*} \int \psi_m \psi_n^{*} dx$$

$$(\lambda_m - \lambda_n^{*}) \int \psi_m \psi_n^{*} dx = 0$$

since $\lambda_n^{*} =$

$$(\lambda_m - \lambda_n) \int \psi_m \psi_n^{*} dx = 0$$ for Hermitic operators

As ~~$(\lambda_m - \lambda_n)$~~ λ_m ad. λ_n ~~and~~ are different, so

$$(\lambda_m - \lambda_n) \neq 0$$

$$\Rightarrow \int \psi_m \psi_n^{*} dx = 0$$

Hence ψ_m and ψ_n are orthogo

Theorem: If λ is degenerate eigenvalue of a Hermitian operator corresponding to linearly independent eigenfunctions $\psi_1, \psi_2, \ldots, \psi_n$, then every linear combination of the same operator corresponding to same eigenvalue.

Proof $\Rightarrow$ Let $\hat{A}$ be a Hermitian operator such that

$$\hat{A}\psi_1 = \lambda \psi_1$$
$$\hat{A}\psi_2 = \lambda \psi_2$$
$$\vdots$$
$$\hat{A}\psi_n = \lambda \psi_n$$

Let us take a linear combination of $\{\psi_i, i = 1, 2, \ldots, n\}$:

$$\Psi = \sum_{i=1}^{n} a_i \psi_i$$

Now

$$\hat{A}\Psi = \hat{A}\left(\sum_{i=1}^{n} a_i \psi_i\right)$$
$$= \sum_{i=1}^{n} a_i \hat{A}\psi_i$$

16-a

$$\hat{A}\Psi = \lambda\left(\sum_{i=1}^{n} a_i \psi_i\right)$$

$$\boxed{\hat{A}\Psi = \lambda\Psi}$$

Hence, Ψ is also an eigenfunction of $\hat{A}$ with eigenvalue ~~A~~ λ.

The Fundamental Commutation Relation

The classical motion of a particle is described in terms of position coordinate "x" and momentum "P_x" along x-direction. In quantum mechanics these observables are replaced with operators

$$x \longrightarrow \hat{x}$$
$$P_x \longrightarrow -i\hbar\frac{\partial}{\partial x}$$

The commutator of operators $\hat{x}$ and momentum "P_x" along ~~x-direction. In quantum mechanics these observables are replaced with operators.~~ is called the fundamental (or canonical) commutation relation

$$[\hat{x}, \hat{P}_x] = i\hbar$$

Similarly

$$[\hat{y}, \hat{P}_y] = i\hbar$$

$$[\hat{z}, \hat{P}_z] = i\hbar.$$

Standard Deviation:

Let us suppose that we have different measurements of the value of x i.e. $x_1, x_2, \ldots, x_N$, for N measurements.

The average value of these measurements is

$$\bar{x} = \frac{x_1 + x_2 + \cdots + x_N}{N}$$

then the deviation of $\bar{x}$ from individual measurements are

$$(x_1 - \bar{x})$$

$$(x_2 - \bar{x})$$

$$\vdots$$

$$(x_N - \bar{x}).$$

17-a Clearly the average of these deviat[ions]

is zero

i.e.

$$\frac{(x_1-\bar{x})+(x_2-\bar{x})+\cdots+(x_N-\bar{x})}{N}$$

$$=\frac{(x_1+x_2+\cdots+x_N)-N\bar{x}}{N}$$

$$=\bar{x}-\bar{x}=0$$

But the mean square of deviations

is in general non-zero.

Now define Δx as positive square r[oot]

of

$$(\Delta x)^2=\frac{(x_1-\bar{x})^2+(x_2-\bar{x})^2+\cdots+(x_N-\bar{x})^2}{N}$$

$$(\Delta x)^2=\frac{x_1^2+x_2^2+\cdots+x_n^2}{N}+\frac{N(\bar{x})^2}{N}$$

$$-\frac{2\bar{x}(x_1+x_2+\cdots+x_N)}{N}$$

$$(\Delta x)^2 = \overline{x^2} + (\bar{x})^2 + 2(\bar{x})^2$$

$$\boxed{(\Delta x)^2 = \overline{x^2} - (\bar{x})^2}$$

In quantum mechanics, the deviation of a reading of an observable $\hat{A}$ from the the expectation value $\langle \hat{A} \rangle$ is represented by an operator

$$\hat{A} - \langle \hat{A} \rangle = \Delta \hat{A}$$

The average of this is zero, i.e.

$$\langle \hat{A} - \langle \hat{A} \rangle \rangle = \langle \hat{A} \rangle - \langle \hat{A} \rangle = 0$$

The mean square of the deviation is

$$(\Delta A)^2 = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle$$

$$= \langle \hat{A}^2 - 2\langle \hat{A} \rangle \hat{A} + \langle \hat{A} \rangle^2 \rangle$$

$$= \langle \hat{A}^2 \rangle - 2\langle \hat{A} \rangle \langle \hat{A} \rangle + \langle \hat{A} \rangle^2$$

$$= \langle \hat{A}^2 \rangle - 2\langle \hat{A} \rangle^2 + \langle \hat{A} \rangle^2$$

$$= \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

18-a

If every measurement of A gives $\langle A \rangle$ then $\Delta A = 0$, but if measurements of A are statistically distributed, then ΔA is positive and is a measure of the width of the distribution, and is known as the standard deviation of the values of A. In quantum mechanics ΔA represents the uncertainty in the measurement of A.

Uncertainty Relation between two operators:

If $\hat{A}$ and $\hat{B}$ are two non-commuting Hermitian operators i.e.

$$[\hat{A}, \hat{B}] = i\hat{C}$$

Then the uncertainties in $\hat{A}$ and $\hat{B}$ are related by

$$\Delta\hat{A}\,\Delta\hat{B} \geq \frac{1}{2}|\langle\hat{C}\rangle|$$

where $\langle\hat{C}\rangle$ is the expectation value of $\hat{C}$

Proof:

Let us define an operator

$$G = A + \lambda B + i\mu B$$

where λ, μ are arbitrary real numbers

The inner product $(G\psi, G\psi)$ is the norm of the function $G\psi$, therefore is +ve definite.

$$\int (G\psi)^* G\psi \, dx \geq 0$$

$\Rightarrow$

$$\int (A + \lambda B + i\mu B)^* \psi^* (A + \lambda B + i\mu B) \psi \, dx$$

$$= \int (A^* + \lambda B^* - i\mu B^*) \psi^* (A + \lambda B + i\mu B) \psi \, dx$$

since $\lambda^* = \lambda$
$\mu^* = \mu$

$$= \int \psi^* (A^\dagger + \lambda B^\dagger - i\mu B^\dagger)(A + \lambda B + i\mu B) \psi \, dx$$

$$= \int \psi^* (A + \lambda B - i\mu B)(A + \lambda B + i\mu B) \psi \, dx$$

$\because$ $A^\dagger = A$
$B^\dagger = B$
Hermitian

19-a

$$= \int \psi^* (A^2 + \underline{\lambda AB} + \underline{i\mu AB} + \underline{\lambda BA} + \lambda^2 B^2 + i\lambda\mu B^2 - \underline{i\mu BA} - i\lambda\mu B^2 - i^2\mu^2 B^2) \psi \, d\tau$$

$$= \int \psi^* (A^2 + \lambda \{A, B\} + i\mu [A, B] + (\lambda^2 + \mu^2) B^2) \psi \, d\tau$$

$$= \int \psi^* (A^2 + \lambda C' - \mu C + (\lambda^2 + \mu^2) B^2) \psi \, d\tau$$

where $C' = AB + BA = \{A, B\}$ Classical poisson's

$iC = AB - BA = [A, B]$

$\Downarrow$ commutator

$i^2 C = i[A, B]$

$-C = i[A, B]$

$\Rightarrow$

$$\langle A^2 \rangle + (\lambda^2 + \mu^2) \langle B^2 \rangle + \lambda \langle C' \rangle - \mu \langle C \rangle$$

If $B\psi \neq 0$, the expression can be written as

$$\langle A^2 \rangle + \langle B^2 \rangle \left(\lambda + \frac{1}{2} \frac{\langle C' \rangle}{\langle B^2 \rangle} \right)^2 + \langle B^2 \rangle \left(\mu - \frac{1}{2} \frac{\langle C' \rangle}{\langle B^2 \rangle} \right)^2 - \frac{1}{4} \frac{\langle C' \rangle^2}{\langle B^2 \rangle} - \frac{1}{4} \frac{\langle C \rangle^2}{\langle B^2 \rangle} \geq 0$$

This inequality holds for every value of λ and μ. We can choose λ and μ in such a way that

$$\lambda + \frac{1}{2}\frac{\langle C' \rangle}{\langle B^2 \rangle} = 0$$

$$\mu - \frac{1}{2}\frac{\langle C' \rangle}{\langle B^2 \rangle} = 0$$

In this case

$$\langle A^2 \rangle \langle B^2 \rangle \geq \frac{1}{4}\left(\langle C \rangle^2 + \langle C' \rangle^2 \right)$$

$$\geq \frac{1}{4} \langle C \rangle^2$$

The uncertainty principle is a relation b/w standard deviation defined as

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle$$

$$= \langle A^2 \rangle - \langle A \rangle^2$$

Now replace

$$A \longrightarrow A - \langle A \rangle$$

$$B \longrightarrow B - \langle B \rangle$$

20-a

The new A and B obey the same commutation relation

$$[A, B] = iC$$

$$\Rightarrow \boxed{\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|}$$

This uncertainty relation Plays an important role in the formalism of quantum mechanics. Its application to Position and momentum operators lead to the Heisenberg uncertainty relation which represent one of the pillars of quantum mechanics.

Dirac Notation:

The vectors of function space are denoted by $|\;\rangle$, Called the ket vectors or simply kets. The state vector ϕ_n is expressed as $|\phi_n\rangle$ or as $|n\rangle$ where the label "n" represents one of more quantum numbers. All the ket vectors of a system form a linear vector space called the ket-space. The scalar product of two state-vectors ϕ_m and ϕ_n denoted by the ket $|\phi_m\rangle$ and $|\phi_n\rangle$, respectively is

$$(\phi_m, \phi_n) = \langle \phi_m | \phi_n \rangle$$

where $\langle \phi_m|$ is called the bra-vector corresponding to the ket vector $|\phi_m\rangle$.

All the bra-vectors of a system form a linear vector space called the bra-space.

also called dual space

The operator equation is

$$A|\psi\rangle = |\chi\rangle$$

also called Hilbert space $\mathcal{H}_1$

i.e. the operation of A on a ket from the left produces an other ket.

Dual space of a vector space is the space of all linear functions on that space.

$y = f(x) = a + bx$

21-a

The expectation value of any operat
A in the state $|\psi\rangle$ is

$$\langle A \rangle = \langle \psi | A | \psi \rangle$$

If A operated on a ket $|\psi\rangle$ from
left such that

$$A|\psi\rangle = \lambda |\psi\rangle$$

then $|\psi\rangle$ is said to be an eigenk
of the operator A corresponding to th
eigenvalue λ.

Let $\{|\phi_n\rangle\}$ be an orthonormal se
of eigenkets i.e.

$$\langle \phi_m | \phi_n \rangle = \delta_{mn}$$

The set is complete if

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle = \sum_n |\phi_n\rangle a_n$$

where

$$\boxed{a_n = \cancel{\sum_n} \langle \phi_n | \psi \rangle}$$

The state $|\psi\rangle$ can also be expressed as (22)

$$|\psi\rangle = \underbrace{\sum_n |\phi_n\rangle\langle\phi_n|}\psi\rangle$$

$$\longrightarrow \sum_n |\phi_n\rangle\langle\phi_n| = 1$$

The inner product of a vector with itself is positive definite

$$\langle\psi|\psi\rangle = \left\langle \sum_n a_n \phi_n \middle| \sum_m a_m \phi_m \right\rangle$$

$$= \sum_{n,m} a_n^* a_m \langle\phi_n|\phi_m\rangle$$

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

$$= \sum_n |a_n|^2 \geq 0, \quad n = m$$

Let us consider the eigenket equation

$$A|\phi_n\rangle = \lambda_n|\phi_n\rangle$$

The equivalent eigenbra equation is

$$\langle\phi_n|A^+ = \lambda_n \langle\phi_n|$$

22-a

The expectation value of A in the n-th state is

$$\langle A\rangle = \langle \phi_n | A | \phi_n\rangle = \lambda_n \langle \phi_n | \phi_n\rangle$$

$$= \lambda_n$$

$$\langle A\rangle = \langle \phi_n | A | \phi_n\rangle = \lambda_n \langle \phi_n | \phi_n\rangle$$

$$= \lambda_n$$

If λ_n is real, the two results can be combined together.

$$\boxed{\langle \phi_n | A \phi_n\rangle = \lambda_n}$$

in the basis $\{|\phi_n\rangle\}$

$$\langle \phi_m | \phi_n\rangle = \delta_{mn}$$

$$\sum_n |\phi_n\rangle\langle \phi_n| = \hat{1}$$

(Completeness)

Let us look at the expression

$$\langle \chi | A | \psi \rangle = \langle \chi | \hat{1} A \hat{1} | \psi \rangle$$

$$= \sum_{n,m} \langle \chi | \phi_n \rangle \langle \phi_n | A | \phi_m \rangle \langle \phi_m | \psi \rangle$$

$$= \sum_{n,m} b_n^* A_{nm} a_m$$

$$= \begin{pmatrix} b_1^* & b_2^* & \cdots \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$= \begin{pmatrix} b_1^* & b_2^* & \cdots \end{pmatrix} \begin{pmatrix} A_{11} a_1 + A_{12} a_2 + \cdots \\ A_{21} a_1 + A_{22} a_2 + \cdots \\ \vdots \end{pmatrix}$$

= number.

$$|\psi\rangle = \hat{1}|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle$$

$$= \sum_n a_n |\phi_n\rangle$$