Unit

Matrix formulation of Quantum mechanics

Matrix Algebra:

Matrix is a Special type of operators generally used in quantum mechanics. This Quantum matrix was developed by Heisenberg in 1924.

Matrix - definition:

A system of numbers arranged in rectangular array or square array of rows and columns is called matrix. In general the matrix can be represented as

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{m1} & a_{m2} & & a_{mn} \end{bmatrix}_{m \times n}$$

Matrix is a vector quantity but it cannot be expressed as in terms of simple number as determinance.

Properties of matrix

1. Two matrices will be equal if they are corresponding components (elements) are equal.

In general, $A = B$ if $A_{ik} = B_{ik}$

2. Two or more linear transformations ~~Successfully~~ Successively applied can be combined into a single linear transformation.

$x'' \xrightarrow{B} x \qquad x_i'' = \sum_{j=1}^{n} B_{ij} x_j'$

$x'' \xrightarrow{A} x \qquad x_i'' = \sum_{k=1}^{n} A_{ik} x_k$

$x'' \rightarrow x_i'' \qquad x_i'' = \sum_{j=1}^{n} B_{ij} x_i' \sum_{l=1}^{n} A_{ik} x_k$

element we get $H^{T*} = \begin{bmatrix} A_{11}^{*} & A_{21}^{*} \\ A_{12}^{*} & A_{22}^{*} \end{bmatrix}$ which is equal to $H^{\dagger}$

A matrix is hermitian (or) self adjoint, if it is equal to its hermitian adjoint. $H = H^{\dagger}$ and it is evidently proved that only square matrices are hermitian

Theorem

* Hermitian adjoint of product of series of matrices is the product of their adjoint, in the reverse order
$\therefore (ABC)^{\dagger} = C^{\dagger}B^{\dagger}A^{\dagger}$.

* The Eigen values of hermitian matrices are all real, If A be a hermitian matrix and u be a eigen vector of A belonging to eigen value λ. $Au = \lambda u$

$$u^{*}Au = \lambda u^{*} u$$
$$u^{*}Au = \lambda^{*} u^{*} u$$
$$0 = (\lambda - \lambda^{*}) u^{*} u$$
$$\boxed{\lambda = \lambda^{*}}$$

Unitary matrix:

A matrix is a unitary, If it is hermitian adjoint is equal to its inverse $\therefore U^{\dagger} = U^{-1}$ (or) if $UU^{\dagger} = 1$ and $U^{\dagger}U = 1$ Unitary matrices of are finite ranks must be square

Hilbert space: Each numerical ... act as a ... n dimensional axis

Now let us define, hilbert space and show, how the operators are represented as matrices. And wave functions as vectors and finally show the connection of various representations with quantum theory and their usefulness in quantum mechanical problems.

Operation on a ket vector from the left with Ω produces another ket vector $\Omega|\beta\rangle = |\beta'\rangle$

operation on a ~~ket~~ bra vector from the right with Ω produces another bra vector $\langle\alpha|\Omega = \langle\alpha''|$ compl.

Matrix element of Ω between the states α and β is a number and can be written as

bra and ket

$$\Omega_{\alpha\beta} = \int \psi_\alpha^* (\vec{r})\, \Omega\, \psi_\beta (\vec{r})\, d^3 r$$

number

$$= (\psi_\alpha, \Omega\psi_\beta) = (\Omega^\dagger \psi_\alpha, \psi_\beta)$$

$$= \langle\alpha|\beta'\rangle = \langle\alpha''|\beta\rangle = \langle\alpha|\Omega|\beta\rangle$$

Ω operate two different btwn two states

Ex: The ~~Scalar~~ p_n Schrodinger equation,

$H\psi_n = E_n \psi_n$ $\quad H\psi_n - E_n\psi_n = 0$ ~~has~~ can be written in braket notation $(H - E_n)|n\rangle = 0$ $\quad \psi_n$ state in wave function operate

$$H_{nm} = \int \psi_n^* H \psi_m\, d^3\vec{r}$$

Same state - normal
diff state orthogonal

$$= (\psi_n, H\psi_m) = \langle n|H|m\rangle$$

The bra vectors are the basis vectors of representation and they form a complete orthogonal set $\langle n|m\rangle = \delta_{mn}$ orthonormality and the closure relation is expressed as $\sum |n\rangle\langle n| = I$ (unit matrix)

According to expansion postulate any arbitrary state vector, may be expressed as a linear combination of base vectors namely $\psi_p = \sum_n a_n \phi_n$.

Dirac's notation, this expansion postulate states any arbitrary ket may be expressed as interms of base ket. Therefore, the new notation for the expansion postulate can be written as $\psi_p = \sum_n a_n \phi_n$ → this equals to

$$|p\rangle = |n\rangle\langle n|p\rangle$$

For ex: if ψ_α, ψ_β are two state vectors then its Norm is defined as

$$(\psi_\alpha \cdot \psi_\beta) = \psi_\alpha^\dagger \psi_\beta = \int \psi_\alpha^*(\vec{r})\, \psi_\beta(\vec{r})\, d^3\vec{r} = 1$$

$E = i\hbar \frac{\partial}{\partial t}$

$P = -i\hbar \frac{\partial}{\partial q}$

that is the inner product of two state vectors $\psi_\alpha\ \psi_\beta$ and its a also a number

when α, β are in same state is equal to Norm] Norm (1)

when the inner product vanishes, the state vectors are said to be Orthogonal (0)

rotate

A unitary transformations from one representation to another corresponds to a rotation of axes in the hillbert space. without chang in state vectors

∴ The matrix element.

Ω - operator operate with two state vectors

$$\psi_\alpha^\dagger \Omega \psi_\beta = (\psi_\alpha\ \Omega \psi_\beta)$$

Then the inner product of state vectors ψ_α and $\Omega\psi_\beta$.

Dirac's bra and ket notations:

The transformation theory develop can be put in to an extremly compact form by making use of a notation, invented by Dirac

We describe a state function represented by as ψ_α or ψ_β and state vector represented by a_α or b_α by a ket or ket vector $|\alpha\rangle$ and the hermitian adjoint state $\psi_\alpha^\dagger$, $\psi_\beta^\dagger$, $a_\alpha^\dagger$ or $b_\alpha^\dagger$ by a bra or bra vector $\langle\alpha|$

$\langle\alpha|H|\alpha\rangle \Rightarrow \psi^\dagger H \psi$

The inner product of two state vectors is written as $\psi_\alpha^\dagger \psi_\beta = \langle\alpha|\beta\rangle$ and is called bra-ket notation which is a number.

A geometrical picture that is often used as a state function such as ψ_α, a_α and b_α as state vector infinite dimensional space called hilbert space. Each dimension corresponds to one of the rows of the one column matrix that describes the state and the component of the state vector along that axis of the hilbert space is numerically equals to the corresponding element of the matrix.

For ex: The Energy representation corresponds to choosing to axes in such a way that a state vector oriented along one of these axes is an eigen state of the hamilton.

Hence Hilbert space is a vector space if it is complex and of countable infinite dimensions such that all infinite series occuring in it or convergent.

The Norm of the State function:

Norm

In Quantum mechanics, a state function ψ represents all physically relevant informations about a physical system at a given instant of time is represented by a vector. Along a direction in the hilbert space.

If ψ represents, a physically realisable state then ψ and constant multiple of ψ both represents the same state.

The arbitrary representatible vector of the ray is usually normalized to 1.

The Norm of the state function is just the square of the length of the corresponding state vector hilbert space.

For ex:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

$\therefore$ Trace $A = A_{11} + A_{22}$

$Tr(AB) = Tr(BA)$

$Tr(AB) = Tr(BA)$

$Tr(B^{-1}AB) = Tr\,ABB^{-1} = Tr\,A \Rightarrow$ Similarity transformation

Transformation matrix

If A is a matrix of order $m \times n$, then the transpose of A is $n \times m$ matrix

Adjoint of a matrix

The adjoint of any square matrix A is obtained by replacing every $(i, j)^{th}$ element of A by the co-factor of i,j^{th} element in $|A|$

Hermitian and Unitary matrix

Home work

For ex:

$$\begin{bmatrix} 1 & -2 & 3 \\ 0 & 2 & -1 \\ -4 & 5 & 2 \end{bmatrix}$$

$adj\,A \quad \frac{1}{|A|}$

$$adj\,A = \begin{bmatrix} 9 & 19 & -4 \\ 4 & 14 & 1 \\ 8 & 3 & 2 \end{bmatrix}$$

Hermitian and Unitary matrix

A matrix is hermitian (or) self adjoint, if it is equal to its hermitian adjoint. Thus, H is a Hermitian matrix, if H is equal to $H^{\dagger}$. (ie) $H = H^{\dagger}$, where $H^{\dagger}$ is hermitian adjoint. The hermitian adjoint $A^{\dagger}$ of the matrix A, is the matrix obtained by interchanging rows and columns and taking the complex conjugate of each element.

So, if A is $\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ then interchanging the rows and columns,

$\begin{bmatrix} A_{11} & A_{21} \\ A_{12} & A_{22} \end{bmatrix}$. and taking complex conjugate of each

Inverse, Singular, non-Singular matrices:

If $AB = 1$ then matrix B is called inverse or reciprocal of A That is B = A (inverse)

(ie) $B = A^{-1}$

$AA^{-1} = 1$ or $A^{-1}A = 1$

$BB^{-1} = 1$

$|A| \neq 0$. That is it determinant does not vanish

AA^{-1} always exist.

A is said to non-singular matrix, if it possess and inverse or its determinant does not vanish

A is said to singular matrix, if it does not posess inverse or its determinant vanishes.

For non singular matrices A, B, C, $(ABC^{-1}) = C^{-1}B^{-1}A^{-1}$

Diagonal matrix:

The diagonal matrix has zero element everywhere except for elements in principle diagonal. Unit matrix is a special case of diagonal matrix,

for example,

$$D = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{bmatrix}$$

$D = D_i \delta_{ij}$ where $\delta_{ij} \begin{Bmatrix} 0 & \text{if} & i \neq j \\ 1 & \text{if} & i = j \end{Bmatrix}$

Two diagonal matrices commute to each other (ie) product of two diagonal matrices is again a diagonal matrix.

Trace of the matrix:

The sum of principal diagonal ~~matrix~~ elements of a square matrix is called trace of the matrix.

But $|C| = |A||B|$

- Associative law of multiplication is given as,

$$A(BC) = (AB)C$$

- Distributive law of matrices is given by,

$$A(B+C) = AB + BC$$

Null and Unit matrices:

The null matrix is defined by the equation $OA = AO = 0$

$$O = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

From which follows that all the elements O are 0, where A is any matrix.

The Unit matrix I is defined by,

$$IA = A \quad (\text{or}) \quad AI = A$$

(i.e) $IA = AI = A$

If A is a Square matrix, then I the unit matrix will also be a Square matrix.

The unit matrix will have unit element along its Principle diagonal. And 0 else where.

The element of I are square to kroncker Symbol

$$\delta_{kl} = 0 \quad \text{if } k \neq l$$

$$\delta_{kl} = 1 \quad \text{if } k = l$$

$$\therefore I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

(ie) $C_{ik} = \sum_{j=1}^{n} B_{ij} A_{ik}$

$x_1'' = \sum_{k=1}^{n} C_{ik} x_k$

$C_{ki} = (BA)_{ki}$

$= \sum_{j=1}^{n} B_{ij} A_{ji}$

Addition of matrix :

The matrices can be summed up if they have same order of rows and columns as A is of order $m \times m$.

Properties of matrix addition:

1. Suppose A, B, C are three matrices of same order $m \times n$. then $A + (B+C) = (A+B) + C$ This is called as associative law of addition of matrices

2. $A + B = B + A$ This law is called as commutative law of addition of matrix

3. $A - B = A + (-B)$

Multiplication of Matrices:

$\lambda A = A \lambda$

Where λ is a scalar quantity. A is a $(m \times n)$ matrix

If A is $(m \times n)$ matrix and B is another Bx $(m \times n)$ matrix then the product of two matrices given by $C = BA$

But in general, $AB \neq BA$.

Generally is not commutative.

- But, if (A,B is equal to BA) $AB = BA$

Then the matrices are said to commutate.

angular momentum matrices - Combination (X) of angular momentum States) - Eigen values of the total angular momentum - clebshgardan coefficient - Recursion relation construction procedure - $J_1 = 1/2$ $j_2 = 1/2$) 10

Unit - V

Approximation methods for Bound states

(I) Stationary Perturbation theory - non degenerate case - first order 243 Perturbation - Evaluation of first order energy 195 - 196 - [evaluation of first order correction to wave function - Zeeman effect without electron spin) - [I PB order 201 Stark effect in hydrogen (ii) 217 atom - variation method : Expectation value of energy - Application to excited 218 States - Ground State of helium atom - Variation of the parameter z.] 10.1 - 10.3, 10.5, 10.-

Text book :

1. Q.M (III edition) Schiff . L. I : Mc Graw Hill, 1968, ISBN - 0 - 07 - 085643-5.

2. Q.M Sathyaprakash & Swati Satya : Kedar Nath Ram Nath & co, 2006.

3. QM, Aruldhas J. prentice - Hall of india, 2002, ISBN 81 - 203 - 1962.

Newton's law of motion

statics + dynamics = Mechanics

1) law → concept of force

2) change of momentum

Physical meanings of matrix elements:

- Expectation value $\frac{\int \psi^* A \psi \, d\tau}{\int \psi^* \psi \, d\tau}$ $\langle A \rangle$ $I|\psi\rangle = |\psi\rangle$
- Eigen value $O|\psi\rangle = 0$

operator

representation of the operator is hermitian operator

bra and ket notation representation of the

simple → bra, ket notation term → matrix

* The diagonal matrix element of an operator which is in the diagonal form are just the eigen values.

* Determining the eigen values of the given operator A, occationaly refer to as solving the eigen value problem for the operator amounts to finding the solution to the eigen value equation.

$$\hat{A}|\phi\rangle = a_\phi |\phi\rangle$$

This is written out in terms of the matrix representation of the operator with respect to some set of orthonormal basis vectors. This eigen value equation is given by,

$$\begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \cdots & \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \end{pmatrix} = a \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \end{pmatrix}$$

* If the operator is not in diagonal form, the diagonal matrix elements are the expection values of operators for states that are normalized.

More generally, comp (real) ordinary

$$\frac{\langle \alpha | \hat{X} | \alpha \rangle}{\langle \alpha | \alpha \rangle}$$ is the expectation value of the operator for the state represented by the normalized ket $|\alpha\rangle$.

6. Dynamic State

$$\psi = \sum_n C_n \psi_n$$

linear combination. $C_n = \int \psi_n^* \psi \, d\tau$.

The relationship btwn Quantum mechanics, operators has helped to present the concepts in the form of some postulates. They are

1. $\hat{A}\psi = a\psi$

State of the system is described by a wave fn $\psi(x, y, z, t)$.

2. Every observable physical property of a system can be characterised by a linear operator. eg. position (A) is characterised by operator $\hat{A}$. (for ex $O \to \hat{O}$)

3. The possible value of any physical quantity of a system are gn by eigen value (a) in the operator equation.

4. When an op $\hat{A}$ is operated on a fn ψ, an average result obtained is gn by

$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \psi^* A \psi \, d\tau}{\int_{-\infty}^{\infty} \psi^* \psi \, d\tau}$$

5. As all the w.fn are time dependent (ie) $\psi(x, y, z, t)$ then its subsequent behaviour should be described by time dependent Schrodinger eqn. which is

$$\frac{-ih}{2\pi} \cdot \frac{\partial \psi(x, y, z, t)}{d\tau} = \hat{H}\psi(x, y, z, t).$$

H - Hamiltonian operator on the system.

$$\therefore \left(i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle\right).$$

1. State of system: The state of any physical system at a gn time can be represented by state vector $|\psi(t)\rangle$ (ket) in Hilbert space.

2. Observables and operators:

observable or dynamical variable

Every physically measurable quantity (for ex O) is known as observable or dynamical variable.

In general, $H_I \neq H_S$, $H_{OH} \neq H_{OS}$ and H'_S, H'_H, H'_I are all different. Differentiation of the first of eqn ② gives for the eqn of motion of $|\alpha_I(t)\rangle$.

uv method 2 ...

we get,

$$i\hbar \frac{d}{dt}|\alpha_I(t)\rangle = -H_{os}\, e^{\frac{iH_{os}t}{\hbar}}|\alpha_S(t)\rangle + i\hbar e^{\frac{iH_{os}t}{\hbar}} \frac{d}{dt}|\alpha_S(t)\rangle$$

$$= -H_{os}|\alpha_I(t)\rangle + e^{\frac{iH_{os}t}{\hbar}} H_S e^{\frac{-iH_{os}t}{\hbar}}|\alpha_I(t)\rangle$$

depends

$$i\hbar \frac{d}{dt}|\alpha_I(t)\rangle = e^{\frac{iH_{os}t}{\hbar}} H'_S\, e^{\frac{-iH_{os}t}{\hbar}}|\alpha_I(t)\rangle \quad -③$$

||ly differentiation of the ③ eqn of ②.

$$\frac{d\Omega_I}{dt} = \frac{\partial \Omega_I}{\partial t} + \frac{1}{i\hbar}[\Omega_I, H_{os}] \qquad H_{os} = H_{oI}$$

depends ong

$$\frac{d\Omega_I}{dt} = \frac{\partial \Omega_I}{\partial t} + \frac{1}{i\hbar}[\Omega_I, H_{oI}] \quad ④$$ ← dynamical

In this picture, the state vector change in accordance with H' and the dynamical variables change in accordance with H_o. This picture is useful, if H' is a small disturbance or perturbation, since the dynamical variable have their unperturbed forms, and the state functions are nearly constant in time.

varies with

dynamical - H_o

avoids

state vector - H' - perturbation

small disturbance

Since p is hermitian, the energy eigen value

$\langle k|H|l\rangle = E_k \langle k|l\rangle$ can be zero. Only if the matrix

elements, $\langle k|p|j\rangle$ and $\langle k|x|j\rangle$ are zero for all j.

Hence became say, the energy eigen values are always posi

Next step is to calculate, the commutator bracket of x w.r.

with H.

$$\left.\begin{aligned} xH - Hx &= \frac{i\hbar p}{m} \\ pH - Hp &= -i\hbar Kx \end{aligned}\right\} \cdot (4)$$

Changing the eqns (4) to dirac's notation,

$$\langle k|x|j\rangle\langle j|H|l\rangle - \langle k|H|j\rangle\langle j|x|l\rangle = (E_l - E_k)\langle k|x|l\rangle$$

$$= \frac{i\hbar}{m}\langle k|p|l\rangle \quad - (5)$$

$$(E_l - E_k)\langle k|p|l\rangle = -i\hbar K\langle k|x|l\rangle \quad - (6)$$

derive (5) and (6)

Eliminating x on both sides. $\langle k|x|l\rangle$

$$(E_l - E_k)\langle k|x|l\rangle = \frac{i\hbar}{m}\langle k|p|l\rangle$$

$$(E_l - E_k)\langle k|p|l\rangle = -i\hbar K\langle k|x|l\rangle.$$

and multiply,

$$(E_l - E_k)^2 \langle k|\cancel{p}|l\rangle = \frac{\hbar^2 K}{m}\langle k|\cancel{p}|l\rangle$$

$$\frac{K}{m} = \omega_c^2$$

$$K = m\omega_c^2$$

$$(E_l - E_k)^2 = \frac{\hbar^2 k}{m}$$

$$\therefore (E_l - E_k) = \pm\hbar\sqrt{K/m}.$$

we know, for a harmonic oscillator.

$$\sqrt{K/m} = \omega_c.$$

c for classical har oscillator.

$$\therefore \underset{\text{eigen value}}{(E_l - E_k)} = \pm\hbar\omega_c. \quad - (7)$$

where ω is angular frequency.

The above relation, ω_c shows the only possible sta are whose eigen values, differ from each other by integral multiples of $\hbar\omega_c$..

Matrix theory of harmonic oscillator:

The one dimensional motion of a point mass attracted to a fixed centre by a force that is proportional to that displacements from that centre proinless. One of the fundamental problem of a classical

Therefore 1D harmonic Oscillator very important for quantum mechanical treatment for problem that is the vibrations of individual atoms, in molecules, and in crystals

And the energy of the harmonic oscillator is given by

$\hbar\omega$

where

ω - is the angle frequency of Vibration.

Hence the force F is equal to $-kx$.

$$F = -kx. \quad \text{(hook's law)}$$

where,

x - displacement

F - Force Potential energy is written as, $V(x) = \frac{1}{2}kx^2$.

Now this system can be treated by matrix theory.

the hamiltonian H of the harmonic oscillator can be written as,

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \quad - (1)$$

where

P - momentum coordinate x - position coordinate P, x are hermitian, bez they are physically measurable dynamical Variable.

we know, the quantum condition,

$$xp - px = i\hbar \quad -(2)$$

Energy representation:

Now our aim is to obtain, the energy eigen values and eigen functions.

Now eqn (1) may be written in Dirac's notation as follows.

$$\langle k|H|l\rangle = E_k \langle k|l\rangle$$

$$= \frac{1}{2m}\langle k|p|j\rangle\langle j|p|l\rangle + \frac{1}{2}K\langle k|x|j\rangle\langle j|x|l\rangle \quad -(3)$$

Now,

$$\langle j|p|l\rangle = \langle l|p^\dagger|j\rangle^* = \langle l|p|j\rangle^*$$ Thus for

(since p is hermitian, $\therefore$ the diagonal elements

Interaction picture:

In the Schrodinger and heisenberg's Picture neither the State vectors nor the dynamical Variables, specifying the physical system in time. But both can be altered, by means of Unitary transformations, $e^{\frac{-iHt}{\hbar}}$ then the two pictures obtained are equally Valid. The quantities that are not altered or the matrix elements of dynamical variable calculated between a Pair of States $(\langle \alpha | \Omega | \beta \rangle)$. This provides a complete theory to arrive at Eigen values, Expectation Values and transition properties. ∴ An especially useful third picture can be specified by dividing the hamiltonian into two parts,

time independent part; time dependent part

$$H = H_0 + H' \quad -(1)$$

where, KE, PE; unperturbed hamiltonian; Perturbed hamiltonian

H_0 does not depend on time explicitly.

(ie) for ex, H_0 may be kinetic energy. $AB \neq BA$

AB - BA; commutate - 1; not commutate - 0

H' may be potential energy.

(or) H_0 may be hamiltonian for a simple potential such as coulumb's field.

H' may be, potential due to the interation with an external electromagnetic field.

Hence, H' depends on time explicitly.

Let us define the interaction picture by the equation,

State vector.

$$|\alpha_I(t)\rangle = e^{\frac{iH_{0s}t}{\hbar}} |\alpha_s(t)\rangle \quad \text{const in time}$$

$$\Omega_I(t) = e^{\frac{iH_{0s}t}{\hbar}} \Omega e^{\frac{-iH_{0s}t}{\hbar}} \quad \Bigg\} -(2)$$

operator

Each dynamic Variable connected to operator

So that interaction. Heisenberg Picture are the same when H' is zero.

$$H_H = H_S$$

$$H_{0I} = H_{0S}$$

There corresponds to a Hermitian operator $\hat{O}$ whose eigen vector form a complete basis

3. Measurement and eigen values of the operator:

Measurement of an observable O is obtained by the action of operator $\hat{O}$, on a state vector $|\psi(t)\rangle$

$\hat{O}|\psi(t)\rangle = a_x |\psi_x\rangle$.

The result of measurement of O on the state vector $|\psi(t)\rangle$ is one of the eigen value a_n.

$|\psi(t)\rangle \rightarrow$ before the measurement

$|\psi_x\rangle \rightarrow$ after measurement.

4. Probablistic outcome of measurements:

Discrete systems measurement observable O of a system in the state $|\psi\rangle$. The probablity of obtaining one of the eigen value a_n of the corresponding operator $\hat{O}$ is written as,

$$P_x = \frac{|\langle\psi_x|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_x|^2}{\langle\psi|\psi\rangle}$$

5. The evolution of systems:

The evolution time of a state vector $|\psi(t)\rangle$ of of a system can be expressed in terms of time dependent Schrodinger eqn.

$$i\hbar \frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle$$

H - Hamiltonian operator

Total energy of the system.

Since $g(x)$ is arbitrary, this and the other commutators may be written as operator equations.

$$\left.\begin{aligned} xp_x - p_x x &= -i\hbar\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right) = i\hbar \\ xp_y - p_y x &= -i\hbar\left(x\frac{\partial}{\partial y} - \frac{\partial}{\partial y}x\right) = 0 \\ xy - yx &= 0 \qquad p_x p_y - p_y p_x = 0 \end{aligned}\right\} - (6)$$

There are in agreement with the classical equations (4) when the substitution (3) is made.

The second observation is that the albebraic properties of the commutator brackets are identical with those of the Poisson brackets. It is readily verified from

$$\{A,B\} \equiv \sum_{i=1}^{f}\left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i}\right)$$

that is

$$\{A,B\} = -\{B,A\} \qquad \{A,c\} = 0 \quad \text{where } c \text{ is a number,}$$

$$\{(A_1 + A_2), B\} = \{A_1, B\} + \{A_2, B\}$$

$$\{A_1 A_2, B\} = \{A_1, B\}A_2 + A_1\{A_2, B\}$$

$$\{A, \{B,C\}\} + \{B, \{C,A\}\} + \{C, \{A,B\}\} = 0$$

The order of possibly noncommuting factors has not been altered. Dirac has shown that the form of the quantum analog of the poisson bracket is determined by eqns (7) to be the right side of (5). The constant $\hbar$ is of course, arbitrary so far as this disussion is concerned.

✻ (✻) Postulates of quantum mechanics

1. $P = |\psi^*\psi|^2 = 1$
2. principle of superposition $\psi = c_1\psi_1 + c_2\psi_2$
3. operator → Energy
   → momentum
4. $\hat{A}$ operator $\hat{A}\psi = O_m\psi$.
5. Expectation value, $\langle A \rangle = \dfrac{\int \psi^* A \psi \, d\tau}{\int \psi^* \psi \, d\tau}$

$$-i\hbar \frac{d}{dt} |\alpha_s(t)\rangle = \langle\alpha_s(t)| H^{\dagger} = \langle\alpha_s(t)| H \quad -② $$

Since H is Hermitian bra

The Solution for above two equations can be easily written.

if H is independent of time let us assume, the solution of the form

The operator $e^{-iHt/\hbar}$ is an infinite, sum of H Power w

Each Power of H Each of which is a dynamical Variable, That can be written as an operator or a Square matrix.

∴ The series as a whole is also dynamical Variable and the operators H is found to the unitary since it is hermitian.

$\therefore e^{\frac{-iHt}{\hbar}}$ is unitary and the Norm of the ket is unchanged. The time rate of change of the matrix element of a dynamical Variable Ω_s in the Schrodinger Picture can be easily found, with the help of eqn ①

$$\frac{d}{dt}\langle\alpha_s(t)|\Omega_s|\beta_s(t)\rangle = \left[\frac{d}{dt}\langle\alpha_s(t)|\right]\Omega_s|\beta_s(t)\rangle +$$

$$\frac{d}{dt}|\alpha_s(t)\rangle = \frac{1}{i\hbar} H |\alpha_s(t)\rangle \qquad \langle\alpha_s(t)|\frac{\partial\Omega_s}{\partial t}|\beta_s(t)\rangle +$$

$$\frac{d}{dt}\langle\alpha_s(t)| = \frac{-1}{i\hbar}\langle\alpha_s(t)|H \qquad \langle\alpha_s(t)|\Omega_s\left[\frac{d}{dt}|\beta_s(t)\rangle\right]$$

dynamical Variable bra, ket

$$= \langle\alpha_s(t)|\frac{\partial\Omega_s}{\partial t}|\beta_s(t)\rangle + \frac{1}{i\hbar}\langle\alpha_s(t)|(\Omega_s H - H\Omega_s)|\beta_s(t)\rangle \quad — ④$$

commutative operator

The first term on RHS, is the change in the matrix element, due to explicit dependents of Ω_s with respect to time

Second term, Change in the State vector with respect to time.

The operator in Second term is a Commutative operator. An interesting thing above eqn ④ is

Ω_S commutes with H and has no explicit dependence of time. $\therefore$ RHS $= 0$. And all matrix elements of Ω_S are constant in time. $\therefore$ the dynamical variable is said to be constant of motion.

Heisenberg's Picture: $|\alpha_H(t)\rangle$ — H - Heisenberg

We know from eqn ③

$$|\alpha_S(t)\rangle = e^{-\frac{iHt}{\hbar}} |\alpha_S(0)\rangle$$

as eqn ③

$$\langle \alpha_S(t)| = \langle \alpha_S(0)| e^{iHt/\hbar}$$

It d... on time

LHS

Now sub eqn ③ in ④

$$\frac{d}{dt} \langle \alpha_S(t)|\Omega_S|\beta_S(t)\rangle$$

$$\frac{d}{dt} \langle \alpha_S(0)| e^{iHt/\hbar} \Omega_S e^{-iHt/\hbar} |\beta_S(0)\rangle$$

H commutes + $e^{iHt/\hbar}$

$$= \langle \alpha_S(0)| e^{+iHt/\hbar} \frac{\partial \Omega_S}{\partial t} e^{-\frac{iHt}{\hbar}} |\beta_S(0)\rangle +$$

$$\frac{1}{i\hbar} \langle \alpha_S(0)| \left[e^{iHt/\hbar} \Omega_S e^{-iHt/\hbar}, H \right] |\beta_S(0)\rangle \quad -⑥$$

We know H is commutes with $e^{\pm iHt/\hbar}$

So let us define, the time independent state vectors through,

$$|\alpha_H(t)\rangle = |\alpha_S(0)\rangle$$

$$= e^{iHt/\hbar} |\alpha_S(t)\rangle \quad -⑦$$

$t = 0$ heisen, Schro } Same

and time dependent dynamical variable through,

$$\Omega_H = e^{iHt/\hbar} \Omega_S e^{-iHt/\hbar} \quad -⑧$$

Unless Ω_S commutes with H, Ω_H depends of time. even if Ω_S has no explicit time dependen[ce]

Here the subscript H represents Heisenberg's Picture.

If $t = 0$, the ket vectors and operators in Schrodinger's picture and heisenberg's picture are the same.

There is a strong resemblance btwn The following two equations.

$$\frac{d\Omega_H}{dt} = \frac{\partial \Omega_H}{\partial t} + \frac{1}{i\hbar}[\Omega_H, H] \quad -(1)$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\} \quad -(2)$$

Of the classical equations of motion. This two eqns suggests that quantum analog Substituting the commutator bracket divided by $i\hbar$ can be found in general by for the Poisson bracket,

$$\{A, B\} \rightarrow \frac{1}{i\hbar}[A, B] \quad -(3)$$

and working with the Heisenberg picture

There are two observations that lend support to the this suggestion. The first concerns the classical conditions for a contact transformation from one set of canonical variables q_i, p_i to another Q_i, P_i

$$\{Q_i, P_j\} = \delta_{ij} \qquad \{Q_i, Q_j\} = 0 \qquad \{P_i, P_j\} = 0 \quad -(4)$$

where the poisson brackets are calculated with respect to the original variables q_i, p_i. We saw a Succesful transition from classical to quantum theory could be made by substituting the differential operator $-i\hbar\left(\frac{\partial}{\partial x}\right)$ for p_x etc. The commutator of x and p_x can then be found by letting it operate on an arbitrary function $g(x)$ of the coordinates.

$$(xp_x - p_x x)\, g(x) = -i\hbar x \frac{\partial g}{\partial x} + i\hbar \frac{\partial}{\partial x}(xg) = i\hbar g(x) \quad -(5)$$

If the time $t = t_0$, then $e^{\pm iHt/\hbar}$ will be replaced by $e^{\frac{\pm iH(t-t_0)}{\hbar}}$

Since $|\Omega_H(t)\rangle$ does not depend on time, the time derivative on the left side of eqn (6) can be taken inside the matrix element and the eqn becomes,

$$\langle \alpha_H | \frac{d\Omega_H}{dt} | \beta_H \rangle = \langle \alpha_H | \frac{\partial \Omega_H}{\partial t} | \beta_H \rangle + \frac{1}{i\hbar} \langle \alpha_H | [\Omega_H, H] | \beta_H \rangle \quad (7)$$

(ie) $\frac{\partial \Omega_H}{\partial t} = e^{iHt/\hbar} \frac{\partial \Omega_S}{\partial t} e^{-iHt/\hbar}$

$\therefore$ The eqn of motion in the heisenberg's picture is can be written as,

$$\frac{d\Omega_H}{dt} = \frac{\partial \Omega_H}{\partial t} + \frac{1}{i\hbar}[\Omega_H, H]$$

Ω_S In ~~heisenberg's~~ schrodinger picture, the dynamical variable are constant in time. and the state vector varies with time.

But in heisenberg's picture (representation), the state vectors are constant in time. and the dynamical variable varies with time.

* Poisson brackets → classical mechanics; commutator brackets → Quantum Mechanics

both same.

Hamiltonian eqn in classical mechanics,

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t}$$

$\{\ \} \rightarrow$ Poisson

f - momentum, position coordinate, may be any other

Heisenberg eqn in quantum mechanics,

$$\frac{d\hat{f}}{dt} = -\frac{i}{\hbar}[\hat{f}, \hat{H}] + \frac{\partial \hat{f}}{\partial t}.$$

$[\ ] \rightarrow$ commutator

Poisson bracket [illegible] q,p transform [illegible] canonical transformation. q - canonical conjugate coordination p - momentum

f, q depends on phase space, time.

using (5) we get,

$$\frac{dF_{mn}}{dt} = \frac{1}{i\hbar}\int\left\{\psi_m^*(FH)\psi_n - \psi_m^*(HF)\psi_n\right\}dq$$

$$= \frac{1}{i\hbar}\int\left\{\psi_m^*(FH - HF)\psi_n\right\}dq + \int\psi_m^*\frac{\partial F}{\partial t}\psi_n\,dq$$

$$\frac{dF_{mn}}{dt} = \frac{1}{i\hbar}\left[F,H\right]_{mn} + \left[\frac{\partial F}{\partial t}\right]_{mn} \quad -(8)$$

This is Heisenberg's form of matrix equation of motion of a dynamical variable.

According to eqn (8), F is a constant of motion of $\frac{dF}{dt} = 0$.

This happens when, $\frac{\partial F}{\partial t} = 0$ which implies F is an explicit function of time. And commutative bracket $[F, H] = 0$ $\therefore$ F commutes with H.

When F is not an explicit function of time, then $\frac{dF}{dt} = \frac{1}{i\hbar}[F, H]$

(7) Matrix representation of wave function

The wave function can be expressed in matrix representation by 3 phase.

to define the eqn of motion

1. Schrodinger's Picture
2. Heisenberg's Picture
3. Interaction Picture.

dynamical variable → func. time

time independent

S - Schrodinger

Schrodinger's picture :

$|\alpha_s(t)\rangle$

Let us consider the time dependent Schrodinger equation $[E\psi = H\psi]$ $i\hbar\frac{\partial\psi}{\partial t} = H\psi$. writing the above equation in terms of time dependent $|\alpha_s(t)\rangle$ (ket) and the hamiltonian H. The equation becomes, $i\hbar\frac{d|\alpha_s(t)\rangle}{dt} = H|\alpha_s(t)\rangle$ (ket) $-(1)$

S - Schrodinger picture

writing the hermitian adjoint eqn of motion, the eqn (1) becomes

* Representation of the operators as matrices makes it possible to introduce in direct fraction hermitian operator.

That is $A^{\dagger} = A$ $\therefore$ the matrix representation of the operator equation is $A|\psi\rangle = |\phi\rangle$.

* Many properties of operators can be expressed in terms of properties of their representation matrices.

$I|\psi\rangle = |\psi\rangle$

$O|\psi\rangle = 0$.

Where I is unit matrix, O is null matrix.

Equation of motion in matrix form:

Let q and p represents the position and momentum vectors. The operator $q = q$.

$$P = \frac{\hbar}{i}\frac{\partial}{\partial q} \Leftarrow \frac{i\hbar}{i^2}\frac{\partial}{\partial q} = -i\hbar\frac{\partial}{\partial q}$$

$$\left.\begin{aligned}[q_i, q_j] &= q_i q_j - q_j q_i = 0 \\ [p_i, p_j] &= p_i p_j - p_j p_i = 0 \\ [q_i, p_j] &= q_i p_j - q_j p_i = i\hbar\delta_{ij}\end{aligned}\right\} -(1)$$

Matrix → commutation bracket

Poisson bracket

considering p and q as matrices, the eqn (1) may be expressed as

$$[q_i, p_j] = 0$$

$$\left.\begin{aligned}[p_i, p_j] &= 0 \\ [q_i, q_j] &= 0\end{aligned}\right\}(i)$$

(2) O - null matrix

I - unit matrix

$$[q_i, p_j] = i\hbar\delta_{ij} \cdot I \rightarrow (ii)$$

In terms of elements, eqn 2(ii) is written as

$$[P_i, q_j]_{mn} = \int \psi_m^* \left\{ q_i \frac{\hbar}{i}\frac{\partial}{\partial q_j} - \frac{\hbar}{i}\frac{\partial}{\partial q_i} q_j \right\} \psi_n \, dq.$$

$$\frac{\hbar}{i} \int \psi_m^* \left\{ q_j \frac{\partial \psi_n}{\partial q_i} - \frac{\partial \psi_n}{\partial q_i} q_j \right\} dq$$

$$= i\hbar \int \psi_m^* \psi_n \, dq$$

$$\left. \begin{array}{ll} = i\hbar\, \delta_{mn} = I & \text{if } i=j \\ = 0 & \text{if } i \neq j \end{array} \right\} - (3)$$

To obtain the eqn of motion for any function (F) of P and T, let us write time dependent Schrodinger eqn.

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad - (4a)$$

write the complex conjugate of above equation,

$$-i\hbar \frac{\partial \psi^*}{\partial t} = H^* \psi^* \quad - (4b)$$

As hamiltonian operator is hermitian, we have,

$$\int \psi^* H \psi \, dq = \int (H^* \psi^*) \psi \, dq. \quad - (5)$$

$p = -i\hbar \frac{\partial}{\partial q}$

$E = i\hbar \nabla$

So, therefore the matrix F_{mn} is defined as,

$$F_{mn} = \int \psi_m^* F^* \psi_n \, dq \quad - (6)$$

differentiate eqn (6), with respect to time, we get

$$\frac{dF_{mn}}{dt} = \int \left\{ \frac{\partial \psi_m^*}{\partial t} F \psi_n + \psi_m^* \frac{\partial F}{\partial t} \psi_n + \psi_m^* F \frac{\partial \psi_n}{\partial t} \right\} dq \quad - (7)$$

we know, time dependent Schrodinger equation,

apply Sch eqn for 1st and 3rd term

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \qquad \frac{d\psi}{dt} = \frac{1}{i\hbar} H\psi$$

$$\therefore \frac{dF_{mn}}{dt} = \int \left[\left\{ \left(-\frac{1}{i\hbar} H^* \psi_m^*\right) F \psi_n + \psi_m^* F \left(\frac{1}{i\hbar} H\psi_n\right) \right\} + \psi_m^* \frac{\partial F}{\partial t} \psi_n \right] dq$$

for II term

$$= \frac{1}{i\hbar} \int \left\{ \psi_m^* (FH)\psi_n - (H^* \psi_m^*) F \psi_n \right\} dq + \int \psi_m^* \frac{\partial F}{\partial t} \psi_n \, dq.$$

Therefore the operator P associated with the dynamical variable is said to be Hermitian. If its average value in any state ψ is real. which implies that the average value of P for the state ψ, is to be real then the expression $\int \psi^* P \psi \, d\tau$ must be real (or) in other words, the imaginary factor must be zero

$$\text{Im} \int \psi^* P \psi \, d\tau = 0$$

For any / arbitrary normalizable ψ.

Equation of motion: operator form

The hamiltonian operator, H has the real eigen value so that it is hermitian also the operator H does not change with time and but it is a function of x_{op} and P_{op} alone the time dependents of the state is contained in the wave function. If the symbol A is defined to mean an operator whose expectation in any state ψ is the time derivative of the expectation of operator A.

Time dependent of ψ is given by Schrodinger equation.

For particle

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \quad - (1)$$

the expectation value, of operator A

$$\langle A \rangle = \frac{\int \psi^* A \psi \, d\tau}{\int \psi^* \psi \, d\tau} = (\psi A, \psi) = \langle \psi^* | A | \psi \rangle$$

$$\frac{d}{dt} \langle A \rangle = \left(\frac{\partial \psi}{\partial t}, A\psi \right) + \left(\psi, A \frac{\partial \psi}{\partial t} \right)$$

$(1) \Rightarrow$

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

$$= \frac{i}{\hbar} \left\{ (H\psi, A\psi) - (\psi - A H\psi) \right\}$$

We know H is a Hermitian operator,

$$\therefore \frac{d}{dt} \langle A \rangle = \frac{i}{\hbar} \left(\psi, (HA - AH)\psi \right)$$

Integrate on both side

$$\dot{A} = \frac{i}{\hbar}[H, A] \quad -(2)$$

That is the time derivative of A is the commutator of H and A multiplied by $i/\hbar$

eqn (2) is called equation of motion of A. In quantum mechanics the equation of motion of a dynamical variable is the equation telling what operator is to be associated with the time derivative of the dynamical variable.

According to eqn (2),

The operator associated with $\dot{x} = \frac{i}{\hbar}[H, x] \quad -(3)$

$$\dot{x} = \frac{i}{\hbar}\left(\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]x - x\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\right)$$

$$= \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 x}{\partial x^2} + x.\cancel{V(x)}\right) + \frac{x\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - x\cancel{V(x)}\Big)$$

$$= \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\left(\frac{\partial^2 x}{\partial x^2} - x\frac{\partial^2}{\partial x^2}\right)\right)$$

$$= \frac{-i\hbar}{\cancel{2}m}\left(\cancel{2}\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial x}$$

$$\dot{x} = \frac{1}{m}\left(-i\hbar\frac{\partial}{\partial x}\right)$$

$$\dot{x} = \frac{p}{m} \quad -(4)$$

If the given system is conservative, H is independent of time

$$\dot{H} = \frac{i}{\hbar}[H, H] \quad -(5)$$

$\dot{H} = 0 \quad \frac{dH}{dt} = 0 \quad \therefore H =$ constant of motion.

so that the energy of So any operator which commutes with the hamiltonian of the system and does not depend explicitly on it. is called 'constant of motion' of the system.