# Quantum Mechanics
# Unit – II

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**UNIT – II-b**

**Exactly Soluble Eigen Value Problems and Matrix Formulation**

Hilbert space - Dirac's Hilbert space - Dirac's Notation - Hermitian Operators - Matrix Representation of Wave functions and Operators- Unitary Transformations- Matrix theory of a linear harmonic oscillator - Equations of Motions - Schroedinger, Heisenberg and Interaction Pictures

# Schrödinger equation

The **Schrödinger equation** is a linear partial differential equation that describes the wave function or state function of a quantum-mechanical system

It is a key result in quantum mechanics, and its discovery was a significant landmark in the development of the subject. The equation is named after Erwin Schrödinger, who postulated the equation in 1925, and published it in 1926, forming the basis for the work that resulted in his Nobel Prize in Physics in 1933.

- The concept of a wave function is a fundamental postulate of quantum mechanics; the wave function defines the state of the system at each spatial position, and time.

- Schrödinger's equation can be derived from the fact that the time-evolution operator must be unitary, and must therefore be generated by the exponential of a self-adjoint operator, which is the quantum Hamiltonian.

We **use operators** in **quantum mechanics** because we see **quantum** effects that exhibit linear superposition of states, and **operators** are the right mathematical objects for dealing with linear superposition. The fundamental idea of **quantum mechanics** is that the state of a system can be the sum of two other possible states.

**Eigenvalues** and **Eigenfunctions**. The wavefunction for a given physical system contains the measurable information about the system. ... *"**Eigenvalue**" comes from the German "Eigenwert" which means proper or characteristic value. "**Eigenfunction**" is from "Eigenfunktion" meaning "proper or characteristic function".

The **wave function Ψ** is a mathematical expression. It carries crucial information about the electron it is associated with: from the **wave function** we obtain the electron's energy, angular momentum, and orbital orientation in the shape of the quantum numbers n, l, and $m_l$.

Fundamental particles, such as electrons, may be described as particles or waves. ... The wave function's symbol is the Greek letter psi, $\Psi$ or $\psi$. The wave function $\Psi$ is a mathematical expression.

The **Schrodinger equation** is used to find the allowed energy levels of quantum mechanical systems (such as atoms, or transistors). The associated wavefunction gives the probability of finding the particle at a certain position. ... The solution to this **equation** is a wave that describes the quantum aspects of a system.

## Postulates of QM:

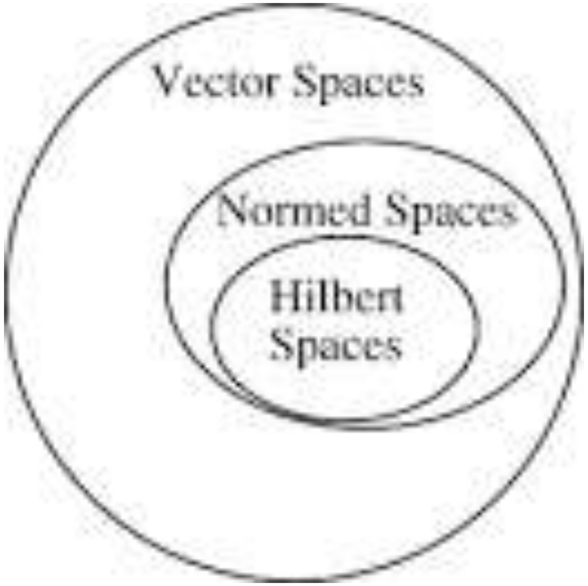
- 1. Wave function
- 2. Operators
- 3. Expectation values
- 4.Eigen Value
- 5. Time development of a quantum system

The **Postulates of Quantum Mechanics**

1. Associated with any particle moving in a conservative field of force is a wave function which determines everything that can be known about the system.

2. The time evolution of the wavefunction is given by the time dependent Schrodinger equation.

A **Hilbert space** is an abstract vector **space** possessing the structure of an inner product that allows length and angle to be measured. Furthermore, **Hilbert spaces are** complete: there **are** enough limits in the **space** to allow the techniques of calculus to be used.



In **quantum mechanics** the state of a physical system is represented by a vector in a **Hilbert space**: a complex vector **space** with an inner product. ◦ The term "**Hilbert space**" is often reserved for an infinite-dimensional inner product **space** having the property that it is complete or closed.

In mathematics, a **Hilbert space** is an inner product **space** that is complete with respect to the norm defined by the inner product. **Hilbert spaces** serve to clarify and generalize the concept of Fourier expansion and certain linear transformations such as the Fourier transform.

**Bra–ket** notation is a notation for linear algebra and linear operators on complex **vector** spaces together with their dual space both in the finite-dimensional and infinite-dimensional case.

In **quantum mechanics**, **Bra-ket** notation is a standard notation for describing **quantum** states, composed of angle brackets and vertical bars. It can also be used to denote abstract vectors and linear functionals in mathematics.

The state of a system can be represented by a vector called *state vector* in the vector space. Dirac introduced the symbol $|\,\rangle$, called the *ket vector* or simply *ket* to denote a state vector which will take different forms in different representations. To distinguish the ket vectors corresponding to different states, a label is introduced in the ket. Thus, the state vector corresponding to $\psi_a(\mathbf{r})$ is denoted by the ket $|a\rangle$. Corresponding to every vector, $|a\rangle$ is defined a conjugate vector $|a\rangle^*$ for which Dirac used the notation $\langle a|$ which is called a *bra vector* or simply *bra*. The conjugate of a ket vector is a bra vector and vice versa. A scalar in the ket space becomes its complex conjugate in the bra space. The bra–ket notation is a distorted form of the *bracket* notation. Thus, the bracket symbol $(\,|\,)$ is distorted to $\langle\,|$ and $|\,\rangle$ in the Dirac notation. The words 'bra' and 'ket' were derived from the word bracket by dropping the letter '*c*'.

- In mathematics, the term "vector" is used for an element of any vector space. In physics, however, the term "vector" is much more specific: "vector" refers almost exclusively to quantities like displacement or velocity, which have components that relate directly to the three dimensions of space, or relativistically, to the four of space time. Such vectors are typically denoted with over arrows

# Bra and ket notation

A wave function $\Psi(\vec{r})$ is a representation of the quantum state $|\Psi\rangle$ in real space. The $|\Psi\rangle$ is called a '**ket**'. At each point ***r*** in space the quantum state $|\Psi\rangle$ is represented by the function $\Psi(\vec{r})$

The quantum state could be expanded in a set of ortho-normal basis states:

$$|\Psi\rangle = \sum_{\phi} |\phi\rangle\langle\phi|\Psi\rangle = \sum_{\phi} C_{\phi}|\phi\rangle$$

Where C's are called expansion coefficients

# Dirac Notation

States can be added to yield a new state ⇒ Superposition

To describe STATES, we use $\overrightarrow{\text{vectors.}}$

VECTORS represent STATES

Each vector can have finite or infinite number of elements

$$\text{DIRAC} \rightarrow \begin{matrix} \textit{bras} & \langle \,| \\ \textit{kets} & |\, \rangle \end{matrix}$$

Each state is denoted by a ket |>. Individual kets are distinguished by the labels placed inside the ket symbol |A>, |B>, etc

A vector has direction and length, and so do the kets

## A state of a dynamical system = direction of ket

Length and sign are irrelevant

# kets

**Multiplication**

$c_i |A\rangle \Rightarrow |A\rangle$

Complex number

**Addition**

we can add two $|\ \rangle$

$|R\rangle = c_1 |A\rangle + c_2 |B\rangle$

many, many $|\ \rangle$

$|R\rangle = \sum_i c_i |L\rangle$

or even have

$|Q\rangle = \int c(x) |X\rangle dx$ if $|x\rangle$ varies continuously

If a state is the superposition of 2 states, then the corresponding ket is the linear combination of 2 other kets

$|\ \rangle$ are independent if no one can be expressed as a linear combination of the others addition of two identical kets

$$c_1|A\rangle + c_2|A\rangle = (c_1 + c_2)|A\rangle \Rightarrow |A\rangle$$

CM: addition of 2 identical states⇒new state

QM: addition of 2 identical states ⇒same state

CM: state can have 0 amplitude (no motion)

QM: |ket> CANNOT have 0 amplitude,

STATE ⇔ direction of vector , and if there is a vector, there is a length.

# bras

To each ket |A>, there corresponds a dual or adjoint quantity called by Dirac a bra; it is not a ket-- rather it exists in a totally different space

a vector that yields a complex number by doing the scalar multiplication with a ket is a:

BRA $\langle \, |$

as it happens with vectors, the scalar product of

$\langle bra || ket \rangle = \langle bra | ket \rangle =$ number

$$\langle B | A \rangle = \sum_{i,j} b_i \cdot a_j$$

$\langle \, |$ have the same properties as $| \, \rangle$,

and are completely defined by their scalar product with every $| \, \rangle$

$$\langle B | \{ | A \rangle + | A' \rangle \} = \underbrace{\langle B | A \rangle}_{number} + \underbrace{\langle B | A' \rangle}_{number}$$

# Operators

An operator is a *rule* that transforms a ket (or bra) in another ket (or bra)
Every observable is associated with an operator

Notation: I use ^ (as most other authors do), Fayer's book uses <u>underline</u>

$$|F\rangle = \hat{\alpha}|A\rangle \qquad \langle G| = \langle B|\hat{\beta}$$

Properties of operators:

- Summation is distributive $\left(\hat{\alpha}+\hat{\beta}\right)|A\rangle = \hat{\alpha}|A\rangle + \hat{\beta}|A\rangle$
- Product is associative $\left(\hat{\alpha}\cdot\hat{\beta}\right)|A\rangle = \hat{\alpha}\left(\hat{\beta}|A\rangle\right)$

ALL Quantum Mechanical operators are LINEAR (not all operators are linear)

Properties of linear operators:

$\hat{\alpha}\left(|A_1\rangle + |A_2\rangle\right) = \hat{\alpha}|A_1\rangle + \hat{\alpha}|A_2\rangle$ and $\hat{\alpha}\mathbb{C}|A\rangle = \mathbb{C}\hat{\alpha}|A\rangle$

# Equations of Motion:

The motion of a physical system can be systematically studied only with the help of equations of motion. If the state is known at a particular time, they allow the determination of the state at a previous or future time. As the state of a physical system is described as fully as possible by a state vector in the vector space, the equation of motion could be an equation for the state vector. State vector as such is not an observable. But the expectation value of a dynamical variable $\langle A \rangle$ is an observable quantity. Therefore, the variation with time of $\langle A \rangle$ can be considered as an equation of motion. The definition of $\langle A \rangle$, Eq. (3.56), suggests that the variation with time of $\langle A \rangle$ may be due to one of the following situations:

1. The state vector changes with time but the operator remains constant (*Schrödinger representation* or *Schrödinger picture*),
2. The operator changes with time while the state vector remains constant (*Heisenberg representation* or *Heisenberg picture*).
3. Both state vector and operator change with time (*interaction representation* or *interaction picture*).

**Thank You Students**