Chapter One

Matrix Formulation of Quantum Mechanics

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Credit goes to students of the 2020-21 session of the Physics department.

Wave and Matrix Mechanics

Wave Mechanics: Wave mechanics is a formulation of quantum mechanics developed by Erwin Schrödinger in 1926. It describes particles, like electrons, as waves rather than point particles.

- The central concept is the wave function (ψ), which contains all the information about a quantum system.
- The behavior of ψ is governed by Schrödinger's equation:

  $$\hat{H}\psi = \mathrm{E}\psi$$

  Where $\hat{H}$ is the Hamiltonian operator, and E is the energy eigenvalue.
- The square of the wave function, $|\psi|^2$ gives the probability density of finding a particle at a certain position.

Matrix Mechanics: Matrix mechanics was developed by Werner Heisenberg, Max Born, and Pascual Jordan in 1925. It was the first complete formulation of quantum mechanics.

- In matrix mechanics, physical quantities (like position, momentum, and energy) are represented by matrices instead of numbers.
- The system's evolution is described using matrix equations rather than differential equations.
- Heisenberg's approach focused on observable quantities and introduced the concept of non-commuting operators, leading to the famous uncertainty principle

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

Relationship and Equivalence

- Schrödinger soon proved that wave mechanics and matrix mechanics are mathematically equivalent—just two representations of the same underlying quantum theory.
- Connection is made via a unitary transformation: in the position basis, operators become differential, yielding wave mechanics; in the energy-eigenstate basis, they become infinite matrices, yielding matrix mechanics.
- Choosing one picture or the other is often a matter of convenience:
  - Wave mechanics is intuitive for spatial problems and potential wells.
  - Matrix/Heisenberg mechanics is compact for spin systems, harmonic oscillators, and time-dependent perturbations.

Quantum State: A quantum state is a mathematical entity that provides a probability distribution for the outcomes of each possible measurement on a system.

Wave function: A wave function in quantum mechanics is a mathematical description of the quantum state of an isolated quantum system. In quantum mechanics, the state of a physical system is represented by a wave function. The most common symbols for a wave function are the Greek letters ψ.

MATRIX REPRESENTATION OF AN OPERATOR

We shall here find the matrix representation of an operator $\hat{A}$. When operator $\hat{A}$ operates on some function *f(x),* the function is transformed into new function *g(x), i.e.,*

$$\hat{A}f(x) = g(x) \qquad \ldots\ldots\ldots (1)$$

It is possible to express the eigenfunctions $f(x)$ and $g(x)$ in terms of a complete orthonormal set of wavefunctions $\psi_n(x)$ operator $\hat{A}$, *i.e.,*

$$f(x) = \sum_m a_m \psi_m (x) \quad and \quad g(x) = \sum_n b_n \psi_n (x) \qquad \ldots\ldots (2)$$

Substituting equation (2) in equation (1), we get,

$$\hat{A} \sum a_m \psi_m (x) = \sum b_n \psi_n (x) \qquad \ldots\ldots..(3)$$

To obtain b_n, We multiply equation (3) by $\psi l^*(x)$ and integrate over the entire space; hence

$$\int \psi_l^*(x)\, \hat{A} \sum_m a_m \psi_m (x) d\tau = \int \psi_l^*(x) \sum_n b_n \psi_n (x) d\tau$$

$$\sum_m a_m \int \psi_l^*(x)\, \hat{A}\psi_m(x) d\tau = \sum_n b_n \int \psi_l^*(x)\, \psi_n(x) d\tau$$

$$\sum_m a_m A_{lm} = \sum_n b_n \delta_{ln} = b_{l,} \qquad \ldots\ldots\ldots(4)$$

Where, $A_{ln} = \int \psi_l^*(x)\, \hat{A}\psi_m(x) d\tau$ ……..(5)

Equation (4) determines the transformation of function *f(x)* into *g(x)* in another representation under the action of the operator $\hat{A}$. The operator $\hat{A}\ in$ this representation is given by equation (5) in the form of a matrix. Thus, the definition of matrix (A) is equivalent to the operator $\hat{A}$ itself. The numbers A_{lm} form a A square array that can be written schematically as

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \ldots & A_{1n} \\ A_{21} & A_{22} & A_{23} & \ldots & A_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & A_{n2} & A_{n3} & \ldots & A_{nn} \end{bmatrix}$$

If the operator $\hat{A}$ is Hermitian, then it may be represented as a diagonal matrix. We know that a Hermitian operator gives real eigenvalues, i.e.,

$$\hat{A}\psi_m = a_m \psi_m$$

From equation (5),

$$A_{lm} = \int \psi_l^*(x) a_m(x)\, \psi_m(x) d\tau = a_m \delta_{lm} \qquad \ldots\ldots\ldots(6)$$

Equation (6) shows that matrix elements with $m = l$ are non-zero, while the elements with $m \neq l$ are zero. Thus, the matrix is diagonal.

$$A=\begin{bmatrix} A_{l1} & 0 & 0 & \dots & 0 \\ 0 & A_{22} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & A_{nn} \end{bmatrix}$$

Thus, each Hermitian operator has a representation as a diagonal matrix, provided the wavefunction is expanded in terms of its eigenfunctions. Hence, the matrix representations of an operator enable us to determine the eigenvalues and eigenfunctions of the corresponding operator. If the operator is known, then the matrix element A_{lm} can be determined. Moreover, if the operator is Hermitian, then it can be represented by a diagonal matrix.

IMPORTANCE OF MATRIX FORMULATION

The importance of the matrix formulation of quantum mechanics, explained below:

1. It provides a precise mathematical language to describe quantum systems using linear algebra.

2. Observables like position, momentum, and energy are represented as matrices (operators), making calculations systematic.

3. The matrix formulation allows computation of measurable quantities like expectation values, eigenvalues, and probabilities.

4. It naturally incorporates the concept of superposition through vector space (Hilbert space).

5. The non-commuting nature of quantum observables (like position and momentum) is easily expressed through matrix multiplication.

6. Time evolution of a quantum state can be described using unitary matrices

7. It links directly with experimental predictions via eigenvalues of operators, which correspond to observable outcomes.

8. Matrix mechanics provides a foundation for quantum computing, where quantum states and gates are represented by matrices.

9. It was the first complete version of quantum mechanics, developed by Heisenberg, Born, and Jordan, before Schrödinger's wave mechanics.

10. Both matrix and wave formulations are mathematically equivalent, but the matrix approach is more suitable in discrete or finite-dimensional systems.

Hermitian Operator

In quantum mechanics and linear algebra, a Hermitian operator is a linear operator that is equal to its Hermitian conjugate (also called adjoint). Mathematically, this is written as:

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

This means that for any two functions or vectors ψ and ϕ in a Hilbert space:

$$< \psi \backslash \hat{A}\, \phi > = \; < \hat{A}\, \psi \backslash \, \phi >$$

Matrix Representation of Hermitian Operator

A Hermitian operator can be represented by a Hermitian matrix when expressed in an orthonormal basis.

A Hermitian matrix is a square matrix that is equal to its conjugate transpose:

$$A = A^{\dagger} = (A^{T})^{*}$$

That is, the diagonal elements are real. The off-diagonal elements are complex conjugates of each other.

Example of a 2×2 Hermitian Matrix:

$$A = \begin{bmatrix} a & c - id \\ c + id & b \end{bmatrix}$$

Where, a, b are real numbers. $c \pm id$ are complex conjugates of each other.

Wave Functions and Eigenvalue Equations

A wave function in quantum mechanics is a mathematical description of the quantum state of an isolated quantum system. In quantum mechanics, the state of a physical system is represented by a wave function. The most common symbols for a wave function are the Greek letters ψ.

Wave Function in Matrix Form

The matrix representation of a wave function ψ arises when we express the state of a system and the operators acting on it in terms of a chosen basis set.

Consider a discrete, complete, and orthonormal basis that is made of a ket set $|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle$

The **orthonormality condition** of the basis ket is expressed by:

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

$$\text{Where } \delta_{nm} = \; 1 \;\; if \; m = n$$

$$= \; 0 \;\; if \; n \neq m$$

The **completeness**, or **closure**, relation for this basis is given by

$$\sum_{n=1}^{\infty} | \, \phi_n \rangle \langle \phi_n \, | \; = \hat{I}$$

The unit operator acts on any ket and leaves it unchanged.

Consider a vector $| \, \psi \rangle$Within the context of the basis set $\{| \, \phi_n \rangle\}$

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_{n=1}^{\infty} |\phi_n\rangle \, \langle \phi_n| \right) |\psi\rangle = \sum_{n=1}^{\infty} a_n |\phi_n\rangle$$

Where $a_n = \langle \phi_n | \psi \rangle$

$$|\psi\rangle \longrightarrow \begin{bmatrix} \langle \phi_1|\psi\rangle \\ \langle \phi_2|\psi\rangle \\ \vdots \\ \langle \phi_n|\psi\rangle \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{bmatrix} \text{ (Ket)}$$

$$\langle \psi| \longrightarrow [\langle \psi|\phi_1\rangle \langle \psi|\phi_2\rangle \dots \langle \psi|\phi_n\rangle \dots] = [\langle \phi_1|\psi\rangle^* \langle \phi_2|\psi\rangle^* \dots \langle \phi_n|\psi\rangle^* \dots] = [a_1^* \, a_2^* \, \dots a_n^* \dots] \text{(Bra)}$$

This is called the matrix form of the wave function, where each entry corresponds to the amplitude of a basis state.

Hence,

$$\langle \psi|\psi\rangle = \sum_n |a_n|^2 = 1$$

Eigenfunction and eigenvalue: Suppose ψ is a well-behaved function of the state of a system, and this is operated on by the operator $\hat{A}$ such that it satisfies the equation,

$$\hat{A}\psi(x) = \lambda\psi(x) \qquad (1)$$

Then the number λ is defined as the eigenvalue of the operator $\hat{A}$ and the operand $\psi(x)$ is an eigenfunction of $\hat{A}$. Equation (1) is termed an eigenvalue equation for the operator $\hat{A}$.

Eigenvalues and Eigenvectors: Let $\hat{A}$ be an $n \times n$ matrix. If there exists a real value λ and a non-zero $n \times 1$ vector $\boldsymbol{x}$ satisfying

$$\hat{A}\,\boldsymbol{x} = \lambda\,\boldsymbol{x} \qquad (2)$$

Then we refer to λ as an eigenvalue of $\hat{A}$, and $\boldsymbol{x}$ is an eigenvector of $\hat{A}$ corresponding to λ.

Moving $\lambda\boldsymbol{x}$ in (2) to the left-hand side gives:

$$\left(\hat{A} - \lambda\hat{I}\right)\boldsymbol{x} = 0 \qquad (3)$$

where $\hat{I}$ is the n × n identity matrix. Introducing $\hat{B} = \hat{A} - \lambda\hat{I}$, We can rewrite the above as

$$\hat{B}\boldsymbol{x} = 0 \qquad (4)$$

Here $\hat{B} = \hat{A} - \lambda\hat{I}$

λ is an eigenvalue only if $Det\left(\hat{B}\right) = 0$

Example: Find eigenvalues and eigenvectors of the matrix $\hat{\boldsymbol{A}} = \begin{bmatrix} \mathbf{1} & \mathbf{0} & \mathbf{-1} \\ \mathbf{1} & \mathbf{2} & \mathbf{1} \\ \mathbf{2} & \mathbf{2} & \mathbf{3} \end{bmatrix}$

Solution:

Let λ be the eigenvalues of the matrix $\hat{A}$. λ is an eigenvalue only if $Det\left(\hat{B}\right) = 0$

$$\hat{B} = \hat{A} - \lambda\hat{I} = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 2 & 2 & 3 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 2 & 2 & 3 \end{bmatrix} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} = \begin{bmatrix} 1-\lambda & 0 & -1 \\ 1 & 2-\lambda & 1 \\ 2 & 2 & 3-\lambda \end{bmatrix}$$

Now, $Det(\hat{B}) = 0$

Or, $\begin{vmatrix} 1-\lambda & 0 & -1 \\ 1 & 2-\lambda & 1 \\ 2 & 2 & 3-\lambda \end{vmatrix} = 0$

Or, $(1-\lambda)[(2-\lambda)\,(3-\lambda)\, -2\,] \,-\, 0 - 1[\,2 -\, 2(2-\lambda)] = 0$

Or, $(1-\lambda)(2-\lambda)(3-\lambda)\, -2\, -2\lambda\, -2+4\, -2\lambda\, = 0$

Or, $(1-\lambda)(2-\lambda)(3-\lambda) = 0$

Hence, eigenvalues are $\lambda = 1, 2, 3$.

When $\lambda = 1$

Let, $\vec{V}(x, y, z)$ be the eigen vectors corresponding values λ.

$Or,\ \hat{B}\ .\vec{V} = 0$

Or, $(\hat{A} - \lambda\hat{I}).\overrightarrow{V} = 0$

Or, $\begin{bmatrix} 0 & 0 & -1 \\ 1 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$

Now, $0 + 0 + Z\ =\ 0$ (1)

$x + y + z = 0$ (2)

$2x + 2y + 2z\ =\ 0$ (3)

By using Cramer's rule in equations (2) and (3)

We have, $x = 0\,, y = 0\ and\ z =\ 0$. Hence, the eigen vector corresponding to $\lambda = 1$ is $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$

Similarly, when $\lambda = 2$

$$\begin{bmatrix} -1 & 0 & -1 \\ 1 & 0 & 1 \\ 2 & 2 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$

$Or, -x + 0 - z = 0$ (4)

$x + 0 + z\ = 0$ (5)

$2x + 2y + z\ = 0$ (6)

from (5) and (6)

$$x = -2\,, y = -1\ and\ z\ =\ 2$$

Hence, the eigen vectors corresponding to $\lambda = 2$ is $\begin{bmatrix} -2 \\ -1 \\ 2 \end{bmatrix}$

When $\lambda\ = 3$

$$\begin{bmatrix} -2 & 0 & -1 \\ 1 & -1 & 1 \\ 2 & 2 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$

$$-2x + 0 - z = 0 \qquad (7)$$

$$x - y + z = 0 \qquad (8)$$

$$2x + xy + z = 0 \qquad (9)$$

We have,

$$x = -1, y = 1 \; and \; z = 2$$

Eigen vectors corresponding to $\lambda = 3$ is $\begin{bmatrix} -1 \\ 1 \\ 2 \end{bmatrix}$

Normalization and Orthogonality of Wavefunction in Matrix Form

The normalization integral of the wavefunction ϕ can be written as

$$\int \phi^* \phi \; d\tau = \int \left(\sum_i c_i^* \psi_i \right) \left(\sum_j c_j \psi_j \right) d\tau$$

$$= \sum_i \sum_j c_i^* c_j \int \psi_i^* \psi_j \; d\tau = \sum_{i\,j} c_i^* c_j \; \delta_{ij}$$

$$= \sum_i c_i^* c_i = \sum_i |c_i|^2$$

and this expresses the square of the length of the magnitude of the vector $\vec{c}$**.** Thus, a normalized wavefunction corresponds to a vector of unit length. In matrix form, we shall write this condition as

$$\int \phi^* \phi \; d\tau = [c_1^* \; c_2^* \; c_3^* \ldots c_n^*] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

$$= C \dagger C = I$$

Similarly, the orthogonality condition for two functions ϕ_a and ϕ_b, viz.

$$\int \phi_a^* \phi_b \; d\tau = 0$$

shall become in matrix form

$$0 = \int \phi_a^* \phi_b \; d\tau = \int \left(\sum_i c_{ai}^* \psi_i * \right) \left(\sum_j c_{bj} \psi_j \right) d\tau$$

$$= \sum_i \sum_j c_{ai}^* c_{bj} \int \psi_i^* \psi_j \, d\tau$$

$$= \sum_{i\ j} c_{ai}^* c_{bj} \, \delta_{ij} = \sum_i c_{ai}^* c_{bi}$$

$$= c_{a1}^* c_{b1} + c_{a2}^* c_{b2} + \cdots + c_{an}^* c_{bn}$$

$$= (c_{a1}^* \ c_{a2}^* \ c_{a3}^* \ldots c_{an}^*) \begin{bmatrix} c_{b1} \\ c_{b2} \\ \vdots \\ c_{bn} \end{bmatrix} = C_a \dagger C_b$$

i.e., the Hermitian scalar product of two vectors must vanish.

Linear Vector Spaces: Hilbert Space

Introduction

We shall now introduce here some terminology that will be useful in the subsequent discussions.

Column vector, Row vector, and Hermitian scalar product

It is conventional to speak of a one-column matrix as a column vector or, simply as a vector. On this analogy, the elements of a column matrix can be visualised as the components of a vector. For the sake of some useful definitions, we take, for example, the column vector x is

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} \qquad (1)$$

To conserve space, we write these elements in a line within curly brackets to represent a column vector:

$$x = \{x^1, x^2, x^3, \ldots, x_n\} \qquad (2)$$

A one-row matrix $[x_1, x_2, x_3 \ldots x_\mathrm{n}]$ will be termed a row vector.

It is obvious that this vector is the transpose of the column vector x.

$$x^\mathrm{T} = [x_1, x_2, \ldots, x_\mathrm{n}] \qquad (3)$$

In a three-dimensional space, $n = 3$, x_1, x_2, x_3 may represent the components of a vector in the directions of a rectangular (x_1, x_2 *and* x_3) axes. The square of the length of this vector is then given by ${x_1}^2 + {x_2}^2 + {x_3}^2$. Extending this definition to a vector in an n-dimensional space, which will now have n −Components, the square of the length of this vector is

$$x^2 = {x_1}^2 + {x_2}^2 + {x_3}^2 + \ldots + {x_\mathrm{n}}^2 \qquad (4)$$

We associate n mutually orthogonal axes with an n-dimensional coordinate system, so that a point has n corresponding coordinates and a vector has n components along these axes. We now, introduce the concept of the scalar product of two vectors in an n −dimensional space. Let the vectors be x and y. The scalar product of x and y is defined by:

$$x^{\mathrm{T}}y \;=\; y^{\mathrm{T}}x \;=\; x_1y_1 \;+\; x_2y_2 \;+\; x_3y_3 + \ldots + x_{\mathrm{n}}y_{\mathrm{n}} \qquad (5)$$

so that if x = y, it also describes the square of the length of the vector x, given by the equation. (4).

When the components of the vectors are complex numbers, we define the *Hermitian scalar* product of a vector x and y as:

$$x^* \dagger y \;=\; x_1^*y_1 \;+ x_2^*y_2 \;+ x_3^*y_3 = \;+ \ldots + x_n^*y_1 \qquad (6)$$

where * denotes complex conjugation. The operation *T is also denoted by the symbol † (dagger). Thus, we have:

$$x \dagger y \;=\; (x^{*T}y) \;=\; (x^T \dagger y^*) * = \; (y^{*T}x)^{*T} \;=\; (y \dagger x) \dagger \qquad (7)$$

Since in a transposition of the product of two matrices, the order of the matrices is reversed. Eq. (7) shows that the two Hermitian scalar products are complex conjugates of each other.

Linear independence of vectors and vector space

A set of n vectors $u_1, u_2, \ldots, u_{\mathrm{n}}$ is said to be linearly independent if there exists no relation between them of the form:

$$c_1u_1 \;+\; c_2u_2 + \ldots + c_{\mathrm{n}}u_{\mathrm{n}} \;=\; 0 \qquad (8)$$

Except when all the c's are zero. For example, in a two-dimensional space, if c_1 and c_2 are not zero, a relation

$$c_1u_1 \;+\; c_2u_2 \;=\; 0$$

$$or, \qquad u_2 \;=\; -(\frac{c_1}{c_2})u_1$$

implies that u_2 is in the direction of u_1. Such two vectors are obviously not linearly independent. For them to be linearly independent, it is necessary that the two be non-collinear, and any two such vectors will define a plane. In a similar way, any three vectors that are not parallel to a plane are linearly independent and constitute a three-dimensional space.

If $u_1, u_2, \ldots, u_{\mathrm{n}}$ are linearly independent vectors in an n-dimensional space, then the set of all y that can be expressed in the form:

$$y \;=\; c_1u_1 \;+\; c_2u_2 + \ldots + c_{\mathrm{n}}u_{\mathrm{n}} \qquad (9)$$

It is called the vector space, spanned by the set of vectors $u_1, u_2, \ldots, u_{\mathrm{n}}$.

We say that the set of n linearly independent vectors forms the basis for the n-dimensional vector space that it spans. Because of the fact that the totality of all vectors y, formed from eq. (9), is obtained as a linear combination of the u −vectors, vector space so defined is also *a linear vector space.*

From eqs. (8) and (9), we can define a linear vector space of n-dimensions if we can find a set of n linearly independent vectors but no such set of $(n+1)$ vectors, for the $(n+1)th$ vector in this space, like y, will be linearly dependent on the u's.

Hilbert Space:

The vector space, suitable for quantum mechanics is called the Hilbert of functional space. To be precise, this is a linear vector space, usually of infinite dimensions and complex, such that all infinite series occurring in it are convergent.

Some definitions of linear vector space.

Basis or basis vector: In an n dimensional space, we may choose a set of n linearly independent vectors, say $\psi_1, \psi_2, \ldots \ldots, \psi_n$. If any arbitrary vector ψ in this space can be expanded in terms of these,

$$\psi = c_1\psi_1 + c_2\psi_2 + \cdots + c_n\psi_n = \sum_{i=1}^{n} c_i\psi_i \qquad (1)$$

then the vectors ψ_i are called basis vectors or a complete set of vectors of the vector space. The coefficients c_i in this expansion may be complex, in general, and are called the components of the vector ψ.

Scalar (Hermitian) product of vectors:

For two vectors $\phi \; and \; \psi$, the (Hermitian) scalar product is defined by:

$$\langle \phi, \psi \rangle = \int \phi^* \psi \, dv = \langle \psi, \phi \rangle^* \qquad (2)$$

DUAL SPACE: DIRAC'S BRA AND KET NOTATION

Now we shall introduce a useful notation due to Dirac, which is commonly used when dealing with scalar products, operators, and state vectors. We shall represent the state vector of the wavefunction ψ by $|\psi\rangle$ and its complex conjugate wavefunction $\psi *$ by $\langle\psi|$. These symbols are referred to as the ket and bra notation, respectively.

The scalar product of two state vectors $|\phi\rangle$ and $|\psi\rangle$ shall become:

$$\langle \phi|\psi\rangle = \int \phi^*(r)\, \psi(r)\, dr$$

The scalar product of two state vectors $|\phi\rangle \; and \; |\psi\rangle$ shall become

$$(\phi, \psi) = \langle \phi|\psi\rangle \qquad (1)$$

in the new notation. Similarly, the matrix elements of the operator $\hat{A}$ will expressed as

$$a_{ij} = \left(\psi_i, \hat{A}\, \psi_j\right) = \langle \psi_i \left| \hat{A} \right| \psi_j \rangle \qquad (2)$$

Also, since $(\phi|\psi) = \langle \psi \, |\phi\rangle *$, (3)

We say that the two spaces, ket $|\,\rangle$ and its complex conjugate bra, $\langle\,|$ are dual to each other, in the sense that, for any complex number λ,

$$\lambda \mid \psi\rangle = |\lambda\psi\rangle \quad (4)$$

But $$\lambda^*\langle \psi| = \langle \lambda\, \psi| \quad (5)$$

The state vectors $|\psi\rangle$ and $\langle\psi|$ are called, respectively, the ket and bra vectors.

Significance of Bra and Ket Notations:

Dirac's bra-ket notation is a symbolic representation introduced by Paul Dirac to simplify the mathematical formulation of quantum mechanics. It plays a vital role in representing quantum states, inner products, and linear operators in a concise and intuitive form.

1. Representation of Quantum States

- A quantum state is written as a ket, for example $|\psi\rangle$ which represents a vector in a complex Hilbert space.
- Its dual vector is represented as a bra, written as $\langle\psi|$, which is the Hermitian conjugate (complex conjugate transpose) of the ket.
- The inner product of two states is written as $\langle\phi|\psi\rangle$.This expression gives the probability amplitude of finding the system in a state $\mid \phi\rangle$ when it is in the state $|\psi\rangle$.
- The square modulus $|\langle\phi|\,\psi\rangle|^2$It gives the probability.
- The outer product, written as $|\psi\rangle\langle\phi|$, represents a linear operator.
- This is often used to define projection operators and is useful in quantum computing and quantum measurements.
- Bra-ket notation simplifies expressions involving basis expansions and linear transformations.
- For example, a quantum state can be expanded as:

$$\mid \psi\rangle = \sum_n c_n \mid n\rangle, \qquad where\ c_n = \langle n \mid \psi\rangle$$

Transformation and diagonalization of matrices:

Let S be a non-singular matrix. Now the similarity trans-formation of a square matrix A into another matrix A' can be written in the form of a transformation equation as

$$S\,A\,S^{-1} = A'$$

$$And \quad S^{-1}\,A'S = A.$$

Any matrix equation remains unaffected by such a transformation.

The following equation

$$AB + CDE = F,$$

can be transformed into

$$SAB\,S^{-1} + SCDE\,S^{-1} = SF\,S^{-1},$$

which is equivalent to

$$SAS^{-1}SBS^{-1} + SCS^{-1}SDS^{-1} \times SES^{-1} = SFS^{-1}$$

$$A'\,B' + C'\,D'\,E' = F' \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where the primes over matrices denote the transformed matrices.

Now we shall illustrate the transformation of a matrix A into

a diagonal matrix D.

$$\text{Let, } A = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \; and \; D = \begin{vmatrix} d_{11} & 0 \\ 0 & d_{22} \end{vmatrix}$$

If the matrix A is transformed to D by the transformation matrix S so that

$$S^{-1}\,AS = D$$

$$or, AS = SD$$

Taking mnth element of both sides, we have

$$\sum_{k=1}^{2} a_{mk}\, s_{kn} = \sum_{k=1}^{2} s_{mk}\, d_{kn} = s_{mn}\, d_{nm}$$

$$a_{m1}s_{1n} + a_{m2}s_{2n} = s_{mn}\, d_{nm}$$

Setting $n = 1$ and $m = 1,2$ we get

$$a_{11}s_{11} + a_{12}s_{2} = s_{11}\, d_{11}$$

$$a_{21}s_{11} + a_{22}s_{21} = s_{21}\, d_{11}$$

This set has the solution for unknown Ss, if the determinant of the coefficient vanishes

$$\begin{vmatrix} a_{11} - d_{11} & a_{12} \\ a_{21} & a_{22} - d_{11} \end{vmatrix} = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Similarly, n=1 and m=1,2 we get

$$\begin{vmatrix} a_{11} - d_{22} & a_{12} \\ a_{21} & a_{22} - d_{22} \end{vmatrix} = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

From equations (2) and (3) we see that d_{11} and d_{22} are the roots of in secular equation in λ

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

When A is a Hermitian matrix, then the secular equation (4) has real roots. Thus, to find the diagonal matrix and consequently the eigenvalues of A, we have to solve the secular equation (4) for A.

Example: reduce to a diagonal form

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & -4 & 2 \\ 0 & 0 & 7 \end{bmatrix}$$

$$\text{Let} \quad A = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -4 & 2 \\ 0 & 0 & 7 \end{bmatrix} \text{ and } l = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

We know that the secular equation is $|A - \lambda l|$=0

$$\left| \begin{bmatrix} 1 & 2 & 3 \\ 0 & -4 & 2 \\ 0 & 0 & 7 \end{bmatrix} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} \right| = \begin{vmatrix} 1-\lambda & 2 & 3 \\ 0 & -4-\lambda & 2 \\ 0 & 0 & 7-\lambda \end{vmatrix} = 0$$

Solving the determinant, we have

$$(1-\lambda)(-4-\lambda)(7-\lambda) = 0$$

$$0\text{r}, \lambda = 1, -4, 7.$$

These are the eigenvalues of matrix A, and the diagonal matrix will be

$$\begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & 7 \end{bmatrix}$$

References:

1 *Quantum Mechanics by Gupta, Kumar, Sharma*

2 (*Internet*)

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