Linear vector space

This module aims at developing the mathematical foundation of Quantum Mechanics, starting from linear vector space and covering topics such as inner product space, Hilbert space, operators in Quantum Mechanics and their matrix representation, postulates of Quantum Mechanics, Heisenberg's uncertainty relation and a particle in a quantum well having infinite potential. These lectures will help the reader to understand the quantum mechanical treatment of optical near fields in a much better way.

In order to define a linear vector space, one has to first define a set of vectors. In this lecture, the Dirac notation for vectors is dealt with.

1 The Dirac notation for vectors in Quantum Mechanics

Any given vector, say $\mathbf{V}$, can be completely defined if and only if all its components are specified. For example, if $\mathbf{e}_i$ are a set of N unit vectors and if v_i are the corresponding N components of $\mathbf{V}$ ($i = 1 \ldots N$), then one can write $\mathbf{V} = \sum_{i=1}^{N} v_i \mathbf{e}_i$. Thus, one can efficiently implement all vector operations, namely, addition, scalar multiplication, etc., in terms of the N components v_i of $\mathbf{V}$. It can be well established that for a given set of unit vectors, the choice of the N components v_i of $\mathbf{V}$ is unique. Hence there exists a one-to-one correspondence between any given vector and its tuple of components such that there exists unique N-tuple of components v_i for each vector $\mathbf{V}$ and vice versa. By exhibiting this unique N-tuple of components v_i into a column vector, one can mathematically represent this correspondence as follows:

$$\mathbf{V} \longleftrightarrow \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}. \tag{1.1}$$

Again, as an adjoint form of Eq.(1.1), $\mathbf{V}$ can also be represented by another distinct N-tuple, namely, the row vector, shown as:

$$\mathbf{V} \longleftrightarrow \begin{pmatrix} v_1^* & v_2^* & \ldots & v_N^* \end{pmatrix}. \tag{1.2}$$

1.1 'Bra' and 'Ket' notations in Quantum Mechanics

In order to identify the aforementioned two distinct forms of the same abstract object $\mathbf{V}$ in Quantum Mechanics, Dirac assigned them as 'Ket V' represented mathematically as $|V\rangle$ and 'Bra V' represented mathematically as $\langle V|$. Hence in Quantum Mechanics, Eq.(1.1) is assigned as $|V\rangle$ ("Ket V") which is represented mathematically as

$$|V\rangle \longleftrightarrow \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}, \tag{1.3}$$

and Eq.(1.2) is assigned as $\langle V|$ ("Bra V") which is represented mathematically as

$$\langle V| \longleftrightarrow \begin{pmatrix} v_1^*, & v_2^*, & \ldots, & v_N^* \end{pmatrix}. \tag{1.4}$$

Thus to each ket, there exists a unique bra and vice versa. More over, if α is any complex constant, then

$$\alpha|V\rangle \longleftrightarrow \begin{pmatrix} \alpha v_1 \\ \alpha v_2 \\ \vdots \\ \alpha v_N \end{pmatrix}, \tag{1.5}$$

and having the corresponding adjoint as

$$\alpha^*\langle V| \longleftrightarrow \begin{pmatrix} \alpha^* v_1^*, & \alpha^* v_2^*, & \ldots, & \alpha^* v_N^* \end{pmatrix}. \tag{1.6}$$

2 Linear vector space

A set of vectors, namely, $\{\ |V_1\rangle,\ \ |V_2\rangle,\ \ |V_3\rangle,\ \ \ldots\ \}$ can constitute a Linear vector space V if and only if they satisfy the following properties such as the set of vectors in V yield only the same vectors in V whenever the operations of addition and scalar multiplication are performed on each and every vector in V, with each vector in V obeying the following axioms given as

- $|V_i\rangle + |V_j\rangle = |V_j\rangle + |V_i\rangle$, known as commutative property of addition,
- $\big(|V_i\rangle + |V_j\rangle\big) + |V_k\rangle = |V_i\rangle + \big(|V_j\rangle + |V_k\rangle\big)$, known as associative property of addition,
- existence of a unique null vector $|\emptyset\rangle$ in V such that $|V_i\rangle + |\emptyset\rangle = |V_i\rangle = |\emptyset\rangle + |V_i\rangle$, thereby existing as an identity element of addition,
- existence of a unique inverse $|-V_i\rangle$ in addition such that $|V_i\rangle + |-V_i\rangle = |\emptyset\rangle$,
- $\alpha\left(|V_i\rangle + |V_j\rangle\right) = \alpha|V_i\rangle + \alpha|V_j\rangle$, pertaining to scalar multiplication,
- $(\alpha + \beta)\,|V_i\rangle = \alpha|V_i\rangle + \beta|V_i\rangle$, also pertaining to scalar multiplication and
- $\alpha\,(\beta|V_i\rangle) = (\alpha\beta)\,|V_i\rangle$, also pertaining to scalar multiplication.

Here, $|V_i\rangle$, $|V_j\rangle$ and $|V_k\rangle$ are arbitrary vectors in the linear vector space V. The linear vector space can be a complex vector space or a real vector space depending on the domain of allowed values of all scalars defined over the linear vector space.

2.1 Linear independence and linear dependence of a set of vectors in a linear vector space

Out of the given set of vectors $\{\ |V_1\rangle,\ \ |V_2\rangle,\ \ \ldots,\ \ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle,\ \ \ldots\ \}$ constituting a linear vector space V, if there exists a linear relation of the form

$$\sum_{j=1}^{N} b_j |j\rangle = |\emptyset\rangle, \tag{2.1}$$

where $|\emptyset\rangle$ is a null vector, and if Eq.(2.1) is satisfied only for the case for which all $b_j = 0$, then such set of vectors $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ are called linear independent vectors. Any other arbitrary vector $|V_j\rangle$ in the linear vector space V that can be expressed as a linear combination of these linear independent vectors represented as

$$|V_j\rangle = \sum_{i=1}^{N} a_i |i\rangle, \tag{2.2}$$

is called a linear dependent vector. The choice of the coefficients a_i is unique for a given set of linear independent vectors.

2.2 Dimensionality of linear vector space

The dimensionality of a linear vector space or linear vector space is decided by the maximum number of linear independent vectors in that linear vector space. Thus if there are at most N number of linear independent vectors, the linear vector space is N dimensional.

3 Basis

For a given set of N linear independent vectors $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ in the linear vector space V, any arbitrary vector $|V_j\rangle$ in the same linear vector space V can be expressed as a linear combination of these N linear independent vectors given by Eq.(2.2). Thus the above mentioned set of N linearly independent vectors is called a basis that spans the linear vector space V. The coefficients a_i in Eq.(2.2) are called the components of the linear dependent vector $|V_j\rangle$ in this basis. In Dirac notation, $|V_j\rangle$ and its adjoint $\langle V_j|$ are represented as follows:

$$\begin{aligned} |V_j\rangle \quad & \xleftrightarrow{\text{in the given basis}} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \qquad \text{and} \\ \langle V_j| \quad & \xleftrightarrow{\text{in the given basis}} \begin{pmatrix} a_1^*, & a_2^*, & \ldots, & a_N^* \end{pmatrix}. \end{aligned} \tag{3.1}$$

4 Inner product

An inner product is the scalar function of any two arbitrary vectors $|V_i\rangle$ and $|V_j\rangle$ taken at a time from a given set of vectors $\{\ |V_1\rangle,\ \ |V_2\rangle,\ \ |V_3\rangle,\ \ \ldots\ \}$ in a linear vector space V and is denoted as $\langle V_i|V_j\rangle$, which evaluates the projection of $|V_j\rangle$ along $|V_i\rangle$. Thus the inner product is a numerical value satisfying the following axioms:

- $\langle V_i|V_i\rangle \geq 0$, pertaining to the positive semi definiteness property,

- $\langle V_i|V_i\rangle = 0$, if and only if $|V_i\rangle = |\emptyset\rangle$, a null vector,
- When $\langle V_i|V_j\rangle = 0$, it means that there is no projection of $|V_j\rangle$ along $|V_i\rangle$. Thus $|V_i\rangle$ and $|V_j\rangle$ are orthogonal to each other.
- $\langle V_i|V_j\rangle = \langle V_j|V_i\rangle^*$, pertaining to the property of skew-symmetry,
- $\langle V_i|\left(\alpha|V_j\rangle + \beta|V_k\rangle\right) \equiv \langle V_i|\left(\alpha V_j + \beta V_k\right)\rangle = \alpha\langle V_i|V_j\rangle + \beta\langle V_i|V_k\rangle$, pertaining to the linearity property in ket and
- $\langle\left(\alpha V_j + \beta V_k\right)|V_i\rangle = \alpha^*\langle V_j|V_i\rangle + \beta^*\langle V_k|V_i\rangle$.

Any vector space consisting of an inner product is called an inner product space or Hilbert space.

5 Norm of a vector

The norm or length of a vector $|V\rangle$ is defined as follows:

$$|V| = \sqrt{\langle V|V\rangle}. \tag{5.1}$$

The unit vector $|i\rangle$ of a vector $|V\rangle$ is defined as follows:

$$|i\rangle \equiv \frac{|V\rangle}{|V|} = \frac{|V\rangle}{\sqrt{\langle V|V\rangle}}, \tag{5.2}$$

where the one-to-one correspondence between $|i\rangle$ and the N-tuple column vector is given as follows:

$$|i\rangle \quad \underset{\text{in the given basis}}{\longleftrightarrow} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{5.3}$$

where "1" is in the i^{th} row of the N-tuple column vector. Also,

$$\langle i| \quad \underset{\text{in the given basis}}{\longleftrightarrow} \begin{pmatrix} 0, & 0, & \ldots, & 0, & 1, & 0, & \ldots, & 0 \end{pmatrix}, \tag{5.4}$$

where "1" is in the i^{th} column of the N-tuple row vector. The norm of this unit vector $|i\rangle$ is then defined as $|i| = \sqrt{\langle i|i\rangle} = 1$. Thus any unit vector has got an unit norm.

6 Orthonormal basis

If the unit vectors of a given set of vectors in the linear vector space V are chosen as the basis vectors, they will be pairwise orthogonal to each other. This is due to the fact that from the given set of unit vectors $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$, the inner product between any two arbitrary unit vectors, namely, $\langle i|j\rangle$ takes the following form:

$$\langle i|j\rangle \equiv \delta_{ij} = \begin{cases} 1 & \text{for} \quad i = j \\ 0 & \text{for} \quad i \neq j, \end{cases} \tag{6.1}$$

where δ_{ij} is the usual Kronecker delta symbol. Hence any given set of unit vectors chosen as the basis vectors form an othonormal basis.

6.1 *Expansion of vectors in an orthonormal basis*

Let $|X\rangle$ be any arbitrary vector in the linear vector space V which can be expressed as linear combination of the N unit vectors, $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ which are chosen as the basis vectors, such that

$$|X\rangle = \sum_{i=1}^{N} x_i |i\rangle, \tag{6.2}$$

where x_i are the N coefficients of $|X\rangle$. The equivalent matrix representation of Eq.(6.2) is given as follows:

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_N \end{pmatrix} = x_1 \begin{pmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \ldots + x_N \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}. \tag{6.3}$$

The projection of $|X\rangle$ along any one of the N unit vectors $|j\rangle$ is given by the inner product $\langle j|X\rangle$, which is evaluated as follows:

$$\begin{aligned} \langle j|X\rangle &= \sum_{i=1}^{N} x_i \langle j|i\rangle, \\ &= \sum_{i=1}^{N} x_i \delta_{ij}, \\ &= x_j, \end{aligned} \tag{6.4}$$

which is the j^{th} coefficient of $|X\rangle$. Thus in order to obtain the i^{th} coefficient x_i of $|X\rangle$, one needs to obtain the inner product $\langle i|X\rangle = x_i$. Hence taking account of Eq.(6.4), $|X\rangle$ can be expressed as follows:

$$|X\rangle = \sum_{i=1}^{N} |i\rangle\langle i|X\rangle. \tag{6.5}$$

Equation (6.5) infers that any arbitrary vector in the given Hilbert space can be expanded in an orthonormal basis. Equations (6.2)-(6.5) show that the best choice of basis vectors are the unit vectors.

Let $|X\rangle$ and $|Y\rangle$ be any two arbitrary vectors in the Hilbert space V which are expressed as linear combination of the N unit vectors, $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ which are chosen as the basis vectors, such that

$$
\begin{aligned}
|X\rangle &= \sum_{i=1}^{N} x_i |i\rangle \quad \text{and} \\
|Y\rangle &= \sum_{j=1}^{N} y_j |j\rangle,
\end{aligned} \tag{6.6}
$$

where x_i are the N coefficients of $|X\rangle$ and y_j are the N coefficients of $|Y\rangle$. Then the inner product between $|X\rangle$ and $|Y\rangle$ is given as follows:

$$
\langle X|Y\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i^* y_j \delta_{ij} = \begin{cases} \sum\limits_{i=1}^{N} x_i^* y_i & \text{for} \quad i = j \\ 0 & \text{for} \quad i \neq j. \end{cases} \tag{6.7}
$$

6.2 Gram-Schmidt theorem for generating an orthonormal basis

Let $\{\ |V_1\rangle,\ \ |V_2\rangle,\ \ |V_3\rangle,\ \ \ldots,\ \ |V_N\rangle\ \}$ be a set of N vectors constituting a Hilbert space V. In order to generate a set of N unit vectors as the orthonormal basis $\{\ |1\rangle,\ \ |2\rangle,\ \ |3\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ from the above mentioned Hilbert space V, the following procedure is employed:

- Let $|1'\rangle = |V_1\rangle$.
- Let $|2'\rangle = |V_2\rangle - \dfrac{|1'\rangle\langle 1'|V_2\rangle}{\langle 1'|1'\rangle}$. Then $\langle 1'|2'\rangle = 0$. As a result, $|1'\rangle$ and $|2'\rangle$ are orthogonal to each other.
- Let $|3'\rangle = |V_3\rangle - \dfrac{|1'\rangle\langle 1'|V_3\rangle}{\langle 1'|1'\rangle} - \dfrac{|2'\rangle\langle 2'|V_3\rangle}{\langle 2'|2'\rangle}$. Then $\langle 1'|3'\rangle = \langle 2'|3'\rangle = 0$.
- Proceeding in this manner, the N^{th} ket can be written as $|N'\rangle = |V_N\rangle - \sum\limits_{i'=1'}^{(N-1)'} \dfrac{|i'\rangle\langle i'|V_N\rangle}{\langle i'|i'\rangle}$, which will be orthogonal to all the previous vectors.
- Thus by following the above mentioned procedure, on finally obtains N orthogonal vectors $\{\ |1'\rangle,\ \ |2'\rangle,\ \ |3'\rangle,\ \ \ldots,\ \ |N'\rangle\ \}$.
- To obtain a set of N orthonormal basis vectors, one needs to evaluate $|i\rangle = \dfrac{|i'\rangle}{\sqrt{\langle i'|i'\rangle}}$, thereby obtaining the N unit vectors $\{\ |1\rangle,\ \ |2\rangle,\ \ \ldots,\ \ |N\rangle\ \}$ as the orthonormal basis vectors.

7 Additional reading and references

1. R. L. Liboff, Introductory Quantum Mechanics (Addison Wesley, New York, 1980).
2. R. Shankar, Principles of Quantum Mechanics (Plenum Press, New York, 1994).
3. D. Ahn and S. H. Park, Engineering Quantum Mechanics (IEEE Press, Singapore, 2011).

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