PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 4, February 04, 2021 (Thursday)

- Reading: Mathematical Tools (Chapter 3 in Griffiths)
- Assignment: Problem Set 2 due February 10 (Wednesday).
  Submit your homework assignments to Canvas.

Topics for Today: Mathematical Tools

2.1 Linear Vector Spaces

2.2 Inner Product and Inner Product Spaces

2.3 Dirac Notation

2.4 Linear Operators

Topics for Next Lecture: Mathematical Tools

2.4 Linear Operators

2.5 Eigenvectors and Eigenvalues

2.6 Expectation Value

2.7 The Uncertainty Principle

2.8 Dirac Delta Functions

2 Mathematical Introduction

2.1 Linear Vector Spaces

Vector

A set of quantities $\{\vec{v}_i\}$ with definite rules for addition and multiplication is called a set of vectors if they satisfy

$$\begin{aligned}
\vec{v}_i + \vec{v}_j &= \vec{v}_j + \vec{v}_i, && (1)\\
\vec{v}_i + (\vec{v}_j + \vec{v}_k) &= (\vec{v}_i + \vec{v}_j) + \vec{v}_k, && (2)\\
\alpha(\vec{v}_i + \vec{v}_j) &= \alpha\vec{v}_i + \alpha\vec{v}_j, && (3)\\
(\alpha + \beta)\vec{v}_i &= \alpha\vec{v}_i + \beta\vec{v}_j, && (4)\\
(\alpha\beta)\vec{v}_i &= \alpha(\beta\vec{v}_i)\,. && (5)
\end{aligned}$$

What is the name of each property?

2.1 Linear Vector Spaces

Vector

A set of quantities $\{\vec{v}_i\}$ with definite rules for addition and multiplication is called a set of vectors if they satisfy

$$
\begin{aligned}
\vec{v}_i + \vec{v}_j &= \vec{v}_j + \vec{v}_i, \ \text{(commutative law of addition)} \\
\vec{v}_i + (\vec{v}_j + \vec{v}_k) &= (\vec{v}_i + \vec{v}_j) + \vec{v}_k, \ \text{(associative law of addition)} \\
\alpha(\vec{v}_i + \vec{v}_j) &= \alpha\vec{v}_i + \alpha\vec{v}_j, \ \text{(distributivity w.r.t vector addition)} \\
(\alpha + \beta)\vec{v}_i &= \alpha\vec{v}_i + \beta\vec{v}_j, \ \text{(distributivity w.r.t number addition)} \\
(\alpha\beta)\vec{v}_i &= \alpha(\beta\vec{v}_i), \ \text{(associative law of multiplication)}
\end{aligned}
$$

where $\alpha, \beta \in \mathcal{C}$ and w.r.t. = 'with respect to'.

Linear Vector Space

If V represents the set of vectors $\{\vec{v}_i\}$ such that

1. $\alpha\vec{v}_i + \beta\vec{v}_j \in V$,
2. there exists a unique null vector or zero vector $\emptyset \in V$ such that $\vec{v}_i + \emptyset = \vec{v}_i = \emptyset + \vec{v}_i$,
3. for every vector $\vec{v}_i$, there exists a unique inverse $-\vec{v}_i \in V$ such that $\vec{v}_i + (-\vec{v}_i) = \emptyset$,

then V is called a linear vector space.

Clearly, the familiar vectors in the 3-dimensional space represent a linear vector space. In that case, addition involves both magnitudes and directions of vectors. The null vector in this case is a vector of zero magnitude and the inverse is a vector with the arrow reversed.

Linear Independence

A set of vectors $\{\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_N\}$ is said to be linearly independent if a relation of the type

$$\sum_{i=1}^{N} \alpha_i \vec{v}_i = 0\,,$$

has the only solution that all α_i's vanish, $\alpha_i = 0$.

Dimensionality

A vector space V is said to be N dimensional, and is denoted by V^N if the maximum number of linearly independent vectors that can be found in that space is N

Theorem

An arbitrary nontrivial vector $\vec{v}$ in V^N can be uniquely expressed as a linear combination of N linearly independent vectors in V^N.

Basis

Any set of linearly independent vectors $\{\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_N\}$ is said to form a basis in V. The coefficients of expansion of any vector $\vec{v}$ in terms of a basis are said to be components in that basis.

Example:

In 3-dimensional vector space, a vector

$$
\begin{aligned}
\vec{x} &= (x_1, x_2, x_3)\,, \\
&= x_1\hat{x} + x_2\hat{y} + x_3\hat{z}\,, \\
&= x_1 e_1 + x_2 e_2 + x_3 e_3\,,
\end{aligned}
$$

where e_i's are linearly independent vectors and form a basis.

2.2 Inner Product and Inner Product Spaces

An inner product is a procedure for assigning a number to two vectors and is denoted by $\langle \vec{v}_i, \vec{v}_j \rangle$. It satisfies the following properties:

(i) $\langle \vec{v}_i, \vec{v}_i \rangle \geq 0$, (0 only if $\vec{v}_i = \emptyset$),

(ii) $\langle \vec{v}_i, \vec{v}_j \rangle = \langle \vec{v}_j, \vec{v}_i \rangle^*$,

(iii) $\langle \vec{v}_i, \alpha \vec{v}_j + \beta \vec{v}_k \rangle = \alpha \langle \vec{v}_i, \vec{v}_j \rangle + \beta \langle \vec{v}_i, \vec{v}_k \rangle$,

If follows from (ii). and (iii). that

$$\begin{aligned}
\langle \alpha \vec{v}_j + \beta \vec{v}_k, \vec{v}_i \rangle &= \langle \vec{v}_i, \alpha \vec{v}_j + \beta \vec{v}_k \rangle^* \\
&= \alpha^* \langle \vec{v}_i, \vec{v}_j \rangle^* + \beta^* \langle \vec{v}_i, \vec{v}_k \rangle^* \\
&= \alpha^* \langle \vec{v}_j, \vec{v}_i \rangle + \beta^* \langle \vec{v}_k, \vec{v}_i \rangle \,.
\end{aligned}$$

Inner Product Space

A vector space with a well-defined inner product is called an inner product space.

Norm

The norm of a vector $\vec{v}$ is defined to be

$$\begin{aligned} v &= |\vec{v}| = \langle \vec{v}, \vec{v} \rangle^{1/2} \\ &= \left(v_1^* v_1 + v_2^* v_2 + \cdots + v_N^* v_N \right)^{1/2} . \end{aligned}$$

And a vector is said to be a unit vector or normalized vector if its norm is one (discrete) or a Dirac delta function (continuous).

Orthogonal

Two vectors are said to be orthogonal if their inner product vanishes,

$$\langle \vec{v}_i, \vec{v}_j \rangle = 0, \quad \text{with} \quad \vec{v}_i, \vec{v}_j \neq \emptyset.$$

Orthonormal

A set of vectors $(e_1, e_2, \cdots, e_N)$ are said to be orthonormal if

$$\langle e_i, e_j \rangle = \delta_{ij}.$$

Let e_i denote an orthonormal basis in V^N, then

$$\begin{aligned} \vec{v} &= \sum_i^N v_i e_i \,, \text{and} \\ \vec{w} &= \sum_i^N w_i e_i \,. \end{aligned}$$

And the inner product becomes

$$\begin{aligned}
\langle \vec{v}, \vec{w} \rangle &= \langle \sum_{i=1}^{N} v_i e_i, \sum_{j=1}^{N} w_j e_j \rangle \,, \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} v_i^* w_j \langle e_i, e_j \rangle \,, \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} v_i^* w_j \delta_{ij} \,, \\
&= \sum_{i=1}^{N} v_i^* w_i \,.
\end{aligned}$$

2.3 Dirac Notation

We realize that an arbitrary vector in V^N can be uniquely expressed in terms of an orthonormal basis $\{|e_i\rangle\}$ as

$$\vec{v} = |v\rangle = \sum_{i=1}^{N} v_i |e_i\rangle.$$

Similarly a vector can be expressed as an ordered n-tuple $(v_1, v_2, \cdots, v_N)$. A familiar example in 3-dimensions is a vector $\vec{x} = (x_1, x_2, x_3)$, where it is assumed that the basis is Cartesian:

$$|\vec{x}\rangle = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad \text{with } |e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \ |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \ |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

where $|e_i\rangle$ are basis vectors.

We can collect the n-tuple into a column vector and obtain

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}, \quad \text{with the basis vectors} \quad |e_i\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}.$$

It is clear that the addition of vectors and multiplication of a vector by a scalar obey matrix formulas with this representation of a vector.

For example,

$$\vec{v} + \vec{w} = \begin{pmatrix} v_1 + w_1 \\ v_2 + w_2 \\ \vdots \\ v_N + w_N \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix} = \vec{z}, \quad \alpha\vec{v} = \begin{pmatrix} \alpha v_1 \\ \alpha v_2 \\ \vdots \\ \alpha v_N \end{pmatrix}.$$

A column representation of a vector is called a **ket vector** and it is denoted by

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}.$$

Given a column vector, we can take the Hermitian conjugate (†) of it and obtain a row vector

$$\langle v| \quad = \quad \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}^{\dagger} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}^{*^{T}} \quad = (v_1^*, v_2^*, \cdots, v_N^*)\,,$$

where $* =$ complex conjugate, and $T =$ transpose.

Obviously, this can also be a representation of $\vec{v}$. It is called a **bra vector** and is denoted by

$$\text{bra}\ \ v = \langle v| = |v\rangle^{\dagger} = (\text{ket}\ \ v)^{\dagger}.$$

This is also called taking the adjoint.

Let us now define the inner product of a bra with a ket,

$$
\begin{aligned}
\langle w|v\rangle &\equiv (w_1^*, w_2^*, \cdots, w_N^*)\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} \\
&= w_1^* v_1 + w_2^* v_2 + \cdots + w_N^* v_N = \sum_{i=1}^{N} w_i^* v_i \,.
\end{aligned}
$$

Since we can expand

$$|v\rangle = \sum_{i=1}^{N} v_i |e_i\rangle$$

where v_i's are numbers (components) and $|e_i\rangle$'s are the basis vectors.

We can define basis ket vector ($|e_i\rangle$) and the dual bra vector ($\langle e_i|$) as

$$
\begin{aligned}
|e_i\rangle &= \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \text{and} \\
\langle e_i| &= (0, 0, \cdots, 1, \cdots, 0)\,.
\end{aligned}
$$

The we can write

$$
\begin{aligned}
|v\rangle &= \sum v_i |e_i\rangle, \;\; \text{and} \\
\langle v| &= \sum v_i^* \langle e_i|.
\end{aligned}
$$

Thus,

$$\begin{aligned}
\langle w|v\rangle &= \sum_{i,j} w_j^* \langle e_j|v_i|e_i\rangle \\
&= \sum_{i,j} w_j^* v_i \langle e_j|e_i\rangle \\
&= \sum_{i,j} w_j^* v_i \delta_{ij} \\
&= \sum_{i} w_i^* v_i \,.
\end{aligned}$$

N.B. $\langle e_j|e_i\rangle = \delta_{ij}$.
This is the orthonormal relation for basis vectors.

In addition, we have

$$\begin{aligned} |v\rangle &= \sum_i v_i |e_i\rangle, \\ \langle e_j|v\rangle &= \sum_i v_i \langle e_j|e_i\rangle = \sum_i v_i \delta_{ij} = v_j \,. \end{aligned}$$

Thus, the components of a vector can be obtained by taking the inner products with the appropriate dual bra basis vectors.

We now have a complete set of orthonormal basis vectors:

$$\begin{aligned} |v\rangle &= \sum_i v_i |e_i\rangle = \sum_i |e_i\rangle v_i = \sum_i |e_i\rangle\langle e_i|v\rangle = C \times |v\rangle \,, \\ \langle e_i|e_j\rangle &= \delta_{ij} \quad \text{(orthonormal relation)} \,, \\ C &= \sum_i |e_i\rangle\langle e_i| = \mathrm{I} \quad \text{(completeness relation)} \,, \end{aligned}$$

where I is the identity matrix or the identity operator.

2.4 Linear Operators

An operator denotes a mathematical operation transforms a vector into another vector. Thus if $|v\rangle$ and $|v'\rangle$ are two ket vectors and if Ω is an operator which takes $|v\rangle$ to $|v'\rangle$, we write

$$\Omega|v\rangle = |v'\rangle$$

That means Ω acting on $|v\rangle$ transforms it to $|v'\rangle$.

Operators can also act on bra vectors to produce other bra vectors,

$$\langle v|\Omega = \langle v''|.$$

However, an operator cannot act on a ket vector to generate a bra vector or vice versa.

Linear operators are operators which obey the following rules:

(i) $\Omega(\alpha|v_i\rangle) = \alpha(\Omega|v_i\rangle)$,

(ii) $\Omega(\alpha|v_i\rangle + \beta|v_j\rangle) = \alpha(\Omega|v_i\rangle) + \beta(\Omega|v_j\rangle)$,

(iii) $(\alpha\langle v_i|)\Omega = (\langle v_i|\Omega)\alpha$,

(iv) $(\alpha\langle v_i| + \beta\langle v_j|)\Omega = (\langle v_i|\Omega)\alpha + (\langle v_j|\Omega)\beta$,

where α and β are scalars.

The simplest linear operator is the identity operator I which leaves every vector invariant. Thus

$$\begin{aligned} I|v\rangle &= |v\rangle, \\ \langle v|I &= \langle v|. \end{aligned}$$

The ket and bra vectors are column and row vectors respectively, the operators would be represented by square matrices with N^2 elements.

A knowledge of the transformation properties of the basis vectors determines the matrix elements of the operator completely. For example, if

$$\begin{aligned} \Omega|e_i\rangle &= |e_i'\rangle, \\ \Omega_{ji} &= \langle e_j|\Omega|e_i\rangle = \langle e_j|e_i'\rangle. \end{aligned}$$

Thus if $|e_i'\rangle$ is known, this implies that all Ω_{ji}'s are known. These are called the matrix elements of the operator Ω in this particular basis. Once the Ω_{ji}'s are known, the transformation of any vector under Ω can be easily found out. For example,

$$\begin{aligned} |v\rangle &= \sum_i v_i|e_i\rangle, \\ \Omega|v\rangle &= |v'\rangle = \sum_i v_i'|e_i\rangle. \end{aligned}$$

Then the transformed components can be obtained as

$$
\begin{aligned}
v_i' &= \langle e_i|\Omega|v\rangle, \\
&= \langle e_i|\Omega| \sum_j v_j |e_j\rangle, \\
&= \sum_j v_j \langle e_i|\Omega|e_j\rangle = \sum_j v_j \Omega_{ij} = \sum_j \Omega_{ij} v_j \,.
\end{aligned}
$$

When two or more operators act on a vector, the order in which they act is important. For example,

$$\Lambda\Omega|v\rangle$$

stands for the operation of Ω on $|v\rangle$ followed by the action of the operator Λ. In general,

$$\Lambda\Omega|v\rangle \neq \Omega\Lambda|v\rangle \,.$$

This is clearly reflected in the fact that matrix multiplication is not commutative. The object

$$\Lambda\Omega - \Omega\Lambda \equiv [\Lambda, \Omega]$$

is called the commutator of Λ with Ω and is in general nonzero. When it vanishes, the operators are said to commute.

We can also define the inverse (Ω^{-1}) of an operator Ω such that the operation of Ω on any vector followed by the inverse leaves the vector unchanged. Thus

$$\begin{aligned} \Omega^{-1}\Omega|v\rangle &= |v\rangle, \\ \Omega^{-1}\Omega &= I = \text{identity operator}. \end{aligned}$$

Example 1: The identity operator

$$
\begin{aligned}
|v\rangle &= \sum v_i |e_i\rangle, \\
v_i &= \langle e_i|v\rangle, \\
\text{Thus,} & \\
|v\rangle &= \sum v_i |e_i\rangle \\
&= \sum |e_i\rangle v_i \\
&= \sum |e_i\rangle\langle e_i|v\rangle = I\ |v\rangle\,, \\
\sum |e_i\rangle\langle e_i| &= I \;=\; \text{identity operator,}\;\; \text{(The completeness relation.)} \\
\langle e_j|I|e_k\rangle &= \langle e_j|(\sum_i |e_i\rangle\langle e_i|)|e_k\rangle \\
&= \sum_i \langle e_j|e_i\rangle\langle e_i|e_k\rangle = \sum_i \delta_{ji}\delta_{ik} = \delta_{jk}\,.
\end{aligned}
$$

Example 2: The projection operator

$$
\begin{aligned}
I &= \sum_i |e_i\rangle\langle e_i| = \sum_i P_i \,, \\
P_i &= |e_i\rangle\langle e_i| \;=\; \text{projection operator} \,, \\
|v\rangle &= \sum_j v_j |e_j\rangle \,, \\
P_i|v\rangle &= \sum_j v_j P_i |e_j\rangle \\
&= \sum_j v_j |e_i\rangle\langle e_i|e_j\rangle \\
&= \sum_j v_j |e_i\rangle \delta_{ij} \\
&= v_i |e_i\rangle \,.
\end{aligned}
$$

Thus, $P_i|v\rangle$ i.e. the projection operator acting on a vector projects out its component.

$$\begin{aligned} P_i P_j &= |e_i\rangle\langle e_i|e_j\rangle\langle e_j| \\ &= |e_i\rangle\delta_{ij}\langle e_j| \\ &= |e_i\rangle\langle e_i|\delta_{ij} \\ &= P_i\delta_{ij}\,. \end{aligned}$$

Physically, what this means is that since P_j projects out the jth component of a vector, operation of P_i following P_j would be zero unless both i and j math. Symbolically, we can write

$$P^2 = P.$$

Operators with such properties are called idempotent operators.

Adjoint of an operator:

If an operator Ω acting on a ket vector $|v\rangle$ gives a new ket vector $|v'\rangle$, then the adjoint of Ω is defined to be that operator which transforms the bra $\langle v|$ to $\langle v'|$,

$$\begin{aligned}
\Omega|v\rangle &= |v'\rangle = |\Omega v\rangle, \\
\langle \Omega v| &= \langle v'| = (|v'\rangle)^\dagger = (\Omega|v\rangle)^\dagger = \langle v|\Omega^\dagger, \\
\Omega^\dagger_{ij} &= \langle e_i|\Omega^\dagger|e_j\rangle \\
&= \langle \Omega e_i|e_j\rangle = \langle e_j|\Omega e_i\rangle^* = \langle e_j|\Omega|e_i\rangle^* = \Omega^*_{ji}
\end{aligned}$$

where $\Omega^\dagger$ is the adjoint of Ω and Ω^*_{ji} is the hermitian conjugate of Ω_{ij}.

Exercise: We can show that the adjoint of a product of operators is the product of the adjoint of the operators in the reversed order

$$(\Omega_1 \Omega_2 \cdots \Omega_N)^\dagger = \Omega_N^\dagger \cdots \Omega_2^\dagger \Omega_1^\dagger$$

Hermitian operators

An operator is Hermitian if it is self adjoint, i.e.,

$$\Omega = \Omega^\dagger$$

An operator is anti-Hermitian if

$$\Omega = -\Omega^\dagger$$

An operator is said to be unitary if

$$\Omega\Omega^\dagger = \Omega^\dagger\Omega = I = \text{identity}$$

This implies that the adjoint of a unitary operator is its inverse.

Exercise: Show that a unitary operator U can be written as

$$U = e^{iH}$$

where H is a Hermitian operator.

Theorem

Unitary operators preserve the inner product between vectors they act on.

Let

$$\begin{aligned} U|v\rangle &= |v'\rangle, \text{ and,} \\ \langle w|U^\dagger &= \langle w'|, \end{aligned}$$

then

$$\langle w'|v'\rangle = \langle w|U^\dagger U|v\rangle = \langle w|I|v\rangle = \langle w|v\rangle.$$