PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 5, February 09, 2021 (Tuesday)

- Handout: Solutions to Problem Set 1.
- 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

2.4 Linear Operators

2.5 Eigenvectors and Eigenvalues

Topics for Next Lecture: Mathematical Tools

2.6 Expectation Value

2.7 The Uncertainty Principle

2.8 Dirac Delta Functions

2.9 Operators in Infinite Dimensions

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

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

2.5 Eigenvectors and Eigenvalues

In general, an operator changes a vector into a new vector

$$\Omega|v\rangle = |v'\rangle\,, \quad \text{(transformation)}\,.$$

If the effect of an operator acting on a vector is to multiply it by a scalar, i.e.,

$$\Omega|v\rangle = \omega|v\rangle\,, \quad \text{(eigenvalue equation)}\,,$$

where ω is a scalar.
Note that

- $|v\rangle$ is an eigenvector of the operator Ω,
- The eigenvalue is ω.
- The normalized eigenvector is

$$|u\rangle = \frac{|v\rangle}{\langle v|v\rangle^{1/2}}\,, \quad \text{or} \quad \vec{u} = \frac{\vec{v}}{|\vec{v}|} = \frac{\vec{v}}{(\vec{v}\cdot\vec{v})^{1/2}}\,.$$

It is clear that we can write the above equation as

$$(\Omega - \omega)|v\rangle = 0.$$

and

$$\begin{aligned} \langle e_i|(\Omega - \omega)|v\rangle &= \sum_j v_j \langle e_i|(\Omega - \omega)|e_j\rangle = 0\,, \quad \text{or} \\ \sum_j (\Omega_{ij} - \omega\delta_{ij})v_j &= 0\,, \quad \text{with} \quad |v\rangle = \sum_j v_j |e_j\rangle\,. \end{aligned}$$

This is a set of homogeneous equations. A nontrivial solution exists if the determinant of the coefficient matrix vanishes, i.e.

$$\det(\Omega_{ij} - \omega\delta_{ij}) = 0\,.$$

In an N-dimensional vector space, it is an Nth order polynomial equation in ω. This is the characteristic equation with N solutions for ω as the eigenvalues of the operator Ω.

Example:

Let us consider an operator in V^3,

$$\Omega = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} .$$

The characteristic equation is

$$\det(\Omega_{ij} - \omega\delta_{ij}) = \det \begin{pmatrix} 1-\omega & 0 & 0 \\ 0 & -\omega & 2 \\ 0 & 2 & -\omega \end{pmatrix} = 0 \, .$$

That leads to

$(1-\omega)(\omega^2 - 4) = 0 \quad \text{or} \quad (\omega - 1)(\omega + 2)(\omega - 2) = 0 \, , \quad \text{with } \omega = 1, 2, -2.$

Let us choose $\omega_1 = 2$, $\omega_2 = 1$, $\omega_3 = -2$ in the descending order.

For $\omega = \omega_1 = 2$, we have

$$\Omega|a\rangle = \omega_1|a\rangle \quad \text{or} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 2 \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

with the eigenvector $|a\rangle$

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} .$$

That leads to three equations

$$a_1 = 2a_1\,, \quad 2a_3 = 2a_2\,, \quad 2a_2 = 2a_3$$

with $a_1 = 0$, $a_3 = a_2$, and a_2 is arbitrary.

Thus the eigenvector corresponding to eigenvalue $\omega_1 = 2$ is

$$|a\rangle = \begin{pmatrix} 0 \\ a_2 \\ a_2 \end{pmatrix}.$$

We can utilize the arbitrariness in a_2 to choose $a_2 \in \mathcal{R}$, $a_2 > 0$ and define a normalized eigenvector

$$|u_1\rangle = |\omega_1\rangle = \frac{|a\rangle}{\sqrt{\langle a|a\rangle}} = \frac{1}{\sqrt{2}a_2} \begin{pmatrix} 0 \\ a_2 \\ a_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

such that $\langle \omega_1|\omega_1\rangle = 1$.

For $\omega = \omega_2 = 1$, we have

$$\Omega|b\rangle = \omega_2|b\rangle \quad \text{or} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

with the eigenvector $|b\rangle$

$$|b\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} .$$

That leads to three equations

$$b_1 = b_1 \,, \quad 2b_3 = b_2 \,, \quad 2b_2 = b_3$$

with $b_2 = 0$, $b_3 = 0$, and b_2 is arbitrary.

Thus the eigenvector corresponding to eigenvalue $\omega_2 = 1$ is

$$|b\rangle = \begin{pmatrix} b_1 \\ 0 \\ 0 \end{pmatrix}.$$

We can utilize the arbitrariness in b_1 to choose $b_1 \in \mathcal{R}$, $b_1 > 0$ and define a normalized eigenvector

$$|u_2\rangle = |\omega_2\rangle = \frac{|b\rangle}{\sqrt{\langle b|b\rangle}} = \frac{1}{b_1}\begin{pmatrix} b_1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

such that $\langle \omega_2|\omega_2\rangle = 1$.

For $\omega = \omega_3 = -2$, we have

$$\Omega|c\rangle = \omega_3|c\rangle \quad \text{or} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = -2 \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

with the eigenvector $|c\rangle$

$$|c\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} .$$

That leads to three equations

$$c_1 = -2c_1 \, , \quad 2c_3 = -2c_2 \, , \quad 2c_2 = -2c_3$$

with $c_1 = 0$, $c_3 = -c_2$, and c_2 is arbitrary.

Thus the eigenvector corresponding to eigenvalue $\omega_3 = -2$ is

$$|c\rangle = \begin{pmatrix} 0 \\ c_2 \\ -c_2 \end{pmatrix}.$$

We can utilize the arbitrariness in c_2 to choose $c_2 \in \mathcal{R}$, $c_2 > 0$ and define a normalized eigenvector

$$|u_3\rangle = |\omega_1\rangle = \frac{|c\rangle}{\sqrt{\langle c|c\rangle}} = \frac{1}{\sqrt{2}c_2}\begin{pmatrix} 0 \\ c_2 \\ -c_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

such that $\langle \omega_3|\omega_3\rangle = 1$.

Summary

The operator Ω has eigenvalues $\omega_1 = 2$, $\omega_2 = 1$, and $\omega_3 = -2$, and normalized eigenvectors

$$|\omega_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad |\omega_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\omega_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}.$$

Since the eigenvectors $|\omega_1\rangle$, $|\omega_2\rangle$, and $|\omega_3\rangle$ form a complete set of orthonormal basis vectors, a unitary matrix U can be built out of these eigenvectors and can be expressed as

$$U = (|\omega_1\rangle|\omega_2\rangle|\omega_3\rangle) = \begin{pmatrix} 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{pmatrix}.$$