

Properties of Commutators and Schroedinger Operators and Applications to Quantum Computing

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Abstract— In this paper we study the properties of Hilbert space operators, commutators and Schroedinger equation. We also explore their applications in quantum physics and explain the links between the abstract mathematics and the reality in the physical sense.

Index Terms—Commutators, Schrödinger equation, IT

I. INTRODUCTION

Hilbert spaces are complete inner product spaces with a lot of interesting properties[2]. Operators on Hilbert spaces are also very interesting with a lot of applications to quantum physics. In this paper, we consider general Hilbert space operators, commutators and Schrödinger equations[1] and explore their applications to quantum mechanics.

II. PRELIMINARIES

Consider some vector which can have complex components to be symbolized by $|a\rangle$.

The dual or conjugate of the vector will be symbolized by $\langle a|$. Thus, $\langle a| = (|a\rangle)^*$.

There is some set of basis vectors that can be multiplied by constant coefficients and added together to give $|a\rangle$.

$$|a\rangle = c_1|x_1\rangle + c_2|x_2\rangle + \dots = \sum_j c_j|x_j\rangle \quad (1.1)$$

The constant c can be complex. The basis vectors form the basis or vector space. There can be one to an infinite number of basis vectors.

As an example, consider a position vector R in three dimensions. We can choose to represent the vector in a variety of vector spaces, each with different basis vectors. Let's use the familiar rectangular vector space with the three basis vectors of i, j, k . We can write R as

$$R = xi + yj + zk = \sum_j c_j x_j \quad (2.2)$$

where $c_1=x, c_2=y, c_3=z$ and $x_1=i, x_2=j, x_3=k$. Notice that the components of the vector are the constants c_j . In Dirac notation, this would become:

$$|R\rangle = \sum_j c_j|x_j\rangle \quad (2.3)$$

This example uses a conventional vector quantity, namely position. But one can extend the concept of vector to include "unconventional" quantities. For instance, a function $\psi = \psi(x)$ can be thought of as a vector. The basis vectors are all of the values of x . The vector ψ has a component $\psi(x)$ for each basis vector. Note that there are an infinite number of basis vectors in this case! We can therefore write an expression for the vector ψ as

$$|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)|x\rangle dx = \int_{-\infty}^{\infty} |x\rangle dx \psi(x) \quad (2.4)$$

Any two vectors in a vector space S satisfy closure under addition and scalar multiplication. Formally, if $|a\rangle, |b\rangle \in S$, then

$$\begin{aligned} |a\rangle + |b\rangle &= |b\rangle + |a\rangle \in S \\ c_1|a\rangle + c_2|b\rangle &\in S \end{aligned} \quad (2.5)$$

We now define an operation between 2 vectors called the scalar product such that the product is a scalar (it can be complex). We also require that if the scalar product is performed between a vector and one of the basis vectors, then the scalar is the coefficient c :

scalar product $\langle b| \bullet |a\rangle = \langle b||a\rangle = \langle b|a\rangle$ so that $\langle b|a\rangle = \text{a number}$

and so that $\langle x_j|a\rangle = c_j$

For ordinary vectors, the scalar product is simply the dot product. Consider our position vector example above. Note that the x -component of vector R can be found by taking the dot product of R with $i=x_1$:

$$x = \mathbf{x}_1 \bullet \mathbf{R} = \langle x_1|R\rangle \quad (2.6)$$

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For a function, then, we can find the value of the function $\psi(x)$ [one of the “components” of “vector” $|\psi\rangle$] by taking the scalar product between x [the basis “vector”] and vector $|\psi\rangle$:

$$\psi(x) = \langle x | \psi \rangle \quad (2.7)$$

Substituting (2.7) into (2.4) gives

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle dx \langle x | \psi \rangle \quad (2.8)$$

and we now have the definition for a unit operator. Examining (2.8) we see that

$$\int_{-\infty}^{\infty} |x\rangle dx \langle x | = 1 \quad (2.9)$$

This unit operator is useful in deriving expressions and in vector algebra as we shall see immediately. What happens if we take the scalar product of two “vectors” that are functions of x ? Let the two functions be $\psi(x)$ and $\phi(x)$. Let the two vectors representing the functions be $|\psi\rangle$ and $|\phi\rangle$. Then the scalar product of the two vectors is $\langle \phi | \psi \rangle$. Let us use the unit operator to write

$$\langle \phi | \psi \rangle = \langle \phi | \left\{ \int_{-\infty}^{\infty} |x\rangle dx \langle x | \right\} | \psi \rangle \quad (2.10)$$

Bringing the two vectors into the integrand gives

$$\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} \langle \phi | x \rangle dx \langle x | \psi \rangle \quad (2.11)$$

Now we have established in (2.7) that we can write $\psi(x) = \langle x | \psi \rangle$ and $\phi(x) = \langle x | \phi \rangle$. Taking the complex conjugate of the second expression gives

$$\phi^*(x) = (\langle x | \phi \rangle)^* = \langle \phi | x \rangle \quad (2.12)$$

so that (2.11) becomes

$$\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} \phi^*(x) \psi(x) dx \quad (2.13)$$

Equation (2.13) tells us how to evaluate the scalar product of two vectors that are functions.

**Notice that the scalar product is written with a bracket and involves two vectors. Because of this, Dirac called $\langle \phi |$ a “bra vector” and $|\psi\rangle$ a “ket vector”. These terms are sometimes still used.*

Properties of Vectors

Now that we have defined vectors and the scalar product, we can list some properties. Note that c is a scalar which can be complex.

$$\begin{aligned} \langle b | c | a \rangle &= c \langle b | a \rangle \\ \langle b | \{ |a\rangle + |a'\rangle \} &= \langle b | a \rangle + \langle b | a' \rangle \\ \langle b | a \rangle &= (\langle a | b \rangle)^* \\ \langle a | a \rangle &\geq 0 \text{ and is real} \\ \langle a | 0 \rangle &= 0 \end{aligned} \quad (2.14)$$

III. BASIC CONCEPTS

These definitions involving the scalar product should look very familiar based on your experience with regular vectors.

$$\text{The magnitude of } |a\rangle = \langle a | a \rangle^{1/2}.$$

$$\text{Vectors } |a\rangle \text{ and } |b\rangle \text{ are orthogonal if } \langle a | b \rangle = 0.$$

Vector $|a\rangle$ is a unit vector if $\langle a | a \rangle = 1$. A unit vector is also called a normalized vector.

Two vectors are orthonormal if they are orthogonal and if they are both normalized.

IV. DIRAC DELTA FUNCTION

While we are discussing vector theory as developed by Dirac, it is interesting to see how he came upon the delta function which bears his name. Consider inserting the unit operator into the bracket expression for the function $\langle \phi | \psi \rangle$ in (2.7):

$$\psi(x) = \langle x | \int_{-\infty}^{\infty} |x'\rangle dx' \langle x' | \psi \rangle = \int_{-\infty}^{\infty} \langle x | x' \rangle dx' \psi(x') \quad (2.15)$$

Notice that we have distinguished x and x' . The unit operator must integrate over all possible values of x' while x is just one of the possible values of x' . Now the left side is the value of ψ at one value of x' ($x'=x$) while the right side involves a sum of the values of ψ at all values of x' . There is no way that this can be true unless the scalar product $\langle x | x' \rangle$ has an interesting property. Namely, $\langle x | x' \rangle = 0$ unless $x=x'$ and if $x=x'$ then the integral of $\langle x | x \rangle$ must give one. Dirac called this strange scalar product the delta function:

$$\langle x | x' \rangle = \delta(x - x') \quad (2.16)$$

where

$$\begin{cases} \delta(x-x') = 0 & \text{for } x' \neq x \\ \int_{-\infty}^{\infty} \delta(x-x') dx' = 1 & \text{for } x' = x \end{cases}$$

V. OPERATOR THEORY

Operators operate on vectors to give other vectors:

$$\hat{A}|a\rangle = |b\rangle \quad (2.17)$$

We will be dealing with linear operators: (i)

$$\hat{A}(|a\rangle + |b\rangle) = \hat{A}|a\rangle + \hat{A}|b\rangle \quad (2.18)$$

(ii)

$$\hat{A}(c|a\rangle) = c\hat{A}|a\rangle$$

VI. SOME PROPERTIES OF OPERATORS

$$\begin{aligned} (\hat{A} + \hat{B})|a\rangle &= \hat{A}|a\rangle + \hat{B}|a\rangle \\ (\hat{A}\hat{B})|a\rangle &\neq \hat{B}\hat{A}|a\rangle \quad \text{*usually} \\ \hat{A}\hat{B}|a\rangle &= \hat{A}\{\hat{B}|a\rangle\} \\ \langle b|\hat{A}|a\rangle &= \langle b|\{\hat{A}|a\rangle\} \end{aligned} \quad (2.19)$$

* Operators usually do not commute. We define the commutator of two operators as

$$\boxed{[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}} \quad (2.20)$$

If the operators do commute, then $[\hat{A}, \hat{B}] = 0$.

It is convenient to define the adjoint of an operator as follows. Operator \hat{A} has an adjoint, denoted by \hat{A}^+ such that

$$(\langle b|\hat{A}|a\rangle)^* = \langle a|\hat{A}^+|b\rangle \quad (2.21)$$

We will say more about the adjoint below.

We have developed a *general* definition of a vector, the scalar product, an operator, and various properties in a purely abstract, mathematical sense. What is the connection to quantum physics? Let us briefly describe the connection.

The quantum states of a physical system are identified as vectors. In practice, this means that the wavefunctions are viewed as function vectors. The components of the vectors are the values of the wavefunctions. The components can change with position and time. This means the function vectors can “point” in different directions as position and time vary. If we fix the time to one value or have a time-independent system, then the basis vectors are the position values x in one dimension.

Dynamic variables (physical quantities of the motion like position, momentum, energy) have corresponding linear operators. These quantities are also referred to as observables since they can be measured or observed. We have already listed these operators in Part 1. We will now simply use our notation of “^” above the operators instead of using curly brackets. For instance, the momentum operator is

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

In classical mechanics, the order of dynamic variables in equations doesn't matter. In quantum mechanics, the order of these variables in equations is very important! This is because of how some of them operate on the wavefunction. Formally, we can say that operators do not generally commute in quantum mechanics. For instance, $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} \neq 0$.

In addition to being linear, the adjoint of an operator of a dynamic variable is equal to the operator ($\hat{A}^+ = \hat{A}$). Such operators are called self-adjoint. For example, the adjoint of the momentum operator is

$$\hat{p}^+ = \hat{p} = -i\hbar \frac{\partial}{\partial x}$$

We can demonstrate this by considering the momentum operator operating on the wavefunction of a free particle. The wavefunction is of the form $\Psi(x,t) = Ae^{i(kx-\omega t)}$. Now

$$\hat{p}|\Psi\rangle = -i\hbar \frac{\partial \Psi}{\partial x} = -i\hbar(ik)Ae^{i(kx-\omega t)} = \hbar k|\Psi\rangle$$

so

$$\langle \Psi|\hat{p}|\Psi\rangle = \langle \Psi|\hbar k|\Psi\rangle = \hbar k \langle \Psi|\Psi\rangle = \hbar k$$

assuming that the wavefunction is normalized. The complex conjugate of this scalar product is simply the scalar product itself:

$$(\langle \Psi|\hat{p}|\Psi\rangle)^* = (\hbar k)^* = \hbar k = \langle \Psi|\hat{p}|\Psi\rangle$$

This fact, combined with the definition of the adjoint as expressed in (2.21), gives

$$\langle \Psi | \hat{p}^+ | \Psi \rangle = (\langle \Psi | \hat{p} | \Psi \rangle)^* = \langle \Psi | \hat{p} | \Psi \rangle$$

This can only be true if $\hat{p}^+ = \hat{p}$, i.e. the operator is self-adjoint. The fact that operators of dynamic variables are self-adjoint can be used in the solving of certain physical systems, as we will see.

Let us examine the result of this connection between mathematics, Dirac notation, and physics in more detail.

We now write a one-dimensional, time-dependent wavefunction $\Psi(x,t)$ as a vector $|\Psi\rangle$. The normalization of the wavefunction is expressed as

$$\langle \Psi | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) dx = 1 \quad (2.22)$$

How do we express an average value of a dynamic variable? We already know how to evaluate it. For example, to find the average value of position x we evaluate the integral

$$\bar{x} = \int_{-\infty}^{\infty} \Psi^* x \Psi dx \quad (2.23)$$

Examine this equation a bit closer. We can view the evaluation of the average as follows: (1) Operate on $|\Psi\rangle$ with the operator \hat{x} . This gives a new vector. (2) Now evaluate the scalar product of this new vector with the conjugate of $|\Psi\rangle$. Thus, in Dirac notation this is written as

$$\bar{x} = \langle \Psi | \hat{x} | \Psi \rangle = \langle x \rangle \quad (2.24)$$

The expression $\langle x \rangle$ is just short-hand for the middle expression and is commonly used.

Can you write the full Dirac notation expression and the integral expression for the average momentum of the particle?

$$\bar{p} = \langle p \rangle = ? \quad (2.25)$$

VII. SCHROEDINGER OPERATORS

We can now express the one-dimensional time-independent Schroedinger equation as

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (2.26)$$

You should verify that this is equivalent to the familiar differential equation version we have been using. In terms of operator theory, this equation says that you operate on a

vector and obtain another vector that is parallel to the first. The resulting vector is just a multiple of the original vector. This original vector and the operator have a very special relationship! Usually, an operator will change the direction of a vector.

In general terms, if $\hat{A}|a\rangle = c|a\rangle$ where c is a number (can be complex) then we call $|a\rangle$ an eigenvector of operator \hat{A} and c the eigenvalue.

Equation (2.26) then is an eigenvalue equation, and since the Hamiltonian is the total energy operator, we call $|\psi\rangle$ the energy eigenvector, $\Psi(x)$ the energy eigenfunction or energy eigenstate, and E the energy eigenvalue. For a physical system in which energy is quantized, there are different eigenstates corresponding to the different energy eigenvalues. More than eigenstate may have the same energy. Such states are called degenerate.

Eigenstates & Measurement

We can now state some postulates about the measurement process in quantum mechanics in relation to the theory we have just developed. We will make these postulates specific to the Hamiltonian and the energy eigenstates and eigenvalues, but they apply to any operator corresponding to a dynamic variable and its associated eigenstates and eigenvectors.

1. If a quantum system is in an eigenstate $|\psi\rangle$ of the operator \hat{H} , then a measurement of the energy will certainly give the eigenvalue E as a result.
2. If the system is in a state such that a measurement of \hat{H} is *certain* to give one particular result then the state is an eigenstate of \hat{H} and the result is the eigenvalue E corresponding to \hat{H} .
3. The result of measuring the energy is one of the energy eigenvalues. If the system was not originally in an eigenstate then the measurement causes the system to "jump" into an eigenstate.
 - Corollary: If a measurement is repeated "immediately" after it is performed, the result must be unchanged. Thus the state to which the system jumped as a result of the first measurement must be an eigenstate with an eigenvalue corresponding to the measured value.
4. Every energy eigenvalue is a possible result of the measurement of the energy.
5. If the energy is measured with the system in a particular state, the eigenstates into which the system may jump due to the measurement are such that the original state is dependent on them, i.e. the original state is a linear combination of the eigenstates.

- Corollary: Since the original state can be any state, every state must be dependent on the eigenstates to which the system may jump. The eigenstates form a complete set of states. An operator whose eigenstates form a complete set is called an observable.
6. Suppose the system is in a state $|\phi\rangle$ (not necessarily an *eigenstate*) and a measurement of the energy is made a large number of times, with the system being put back into the original state after each measurement. Then, the average of all of those measurements is $\langle E \rangle = \langle \phi | \hat{H} | \phi \rangle$ assuming that $|\phi\rangle$ is normalized.

REFERENCES

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