21.1: Operators in Quantum Mechanics

The central concept in this new framework of quantum mechanics is that every observable (i.e., any quantity that can be measured in a physical experiment) is associated with an operator. To distinguish between classical mechanics operators and quantum mechanical ones, we use a hat symbol $\hat{}$ on top of the latter. Physical pure states in quantum mechanics are represented as unit-norm (probabilities are normalized to one) vectors in a special complex Hilbert space. Following the definition, an operator is a function that projects a vector in the Hilbert space onto the space of physical observables. Since observables are values that come up as the result of the experiment, quantum mechanical operators must yield real eigenvalues.[16] Operators that possess this property are called **Hermitian**. In the wave mechanics formulation of quantum mechanics that we have seen so far, the wave function varies with space and time—or equivalently momentum and time—and observables are differential operators. A completely analogous formulation is possible in terms of matrices. In the matrix formulation of quantum mechanics, the norm of the physical state should stay fixed, so the evolution operator should be unitary, and the operators can be represented as matrices.

The expectation value of an operator $\hat{A}$ for a system with wave function $\psi(\mathbf{r})$ living in a Hilbert space with unit vector $\mathbf{r}$ (i.e., in three-dimensional Cartesian space $\mathbf{r}=\{x,y,z\}$), is given by:

$$\langle A\rangle=\int\psi^*(\mathbf{r})\hat{A}\psi(\mathbf{r})d\mathbf{r}, \tag{21.1.1}$$

and if $\hat{A}$ is a Hermitian operator, all physical observables are represented by such expectation values. It is easy to show that if $\hat{A}$ is a linear operator with an eigenfunction g, then any multiple of g is also an eigenfunction of $\hat{A}$.

Basic Properties of Operators

Most of the properties of operators are obvious, but they are summarized below for completeness. The sum and difference of two operators $\hat{A}$ and $\hat{B}$ are given by:

$$\begin{aligned}(\hat{A}+\hat{B})f&=\hat{A}f+\hat{B}f\\(\hat{A}-\hat{B})f&=\hat{A}f-\hat{B}f.\end{aligned} \tag{21.1.2}$$

The product of two operators is defined by:

$$\hat{A}\hat{B}f\equiv\hat{A}[\hat{B}f] \tag{21.1.3}$$

Two operators are equal if

$$\hat{A}f=\hat{B}f \tag{21.1.4}$$

for all functions f. The identity operator $\hat{1}$ does nothing (or multiplies by 1):

$$\hat{1}f=f \tag{21.1.5}$$

The associative law holds for operators:

$$\hat{A}(\hat{B}\hat{C})=(\hat{A}\hat{B})\hat{C} \tag{21.1.6}$$

The commutative law does not generally hold for operators. In general, $\hat{A}\hat{B}\neq\hat{B}\hat{A}$. It is convenient to define the quantity:

$$[\hat{A},\hat{B}]\equiv\hat{A}\hat{B}-\hat{B}\hat{A} \tag{21.1.7}$$

which is called the **commutator** of $\hat{A}$ and $\hat{B}$. Note that the order matters, so that $[\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$. If $\hat{A}$ and $\hat{B}$ happen to commute, then $[\hat{A},\hat{B}]=0$.

Linear Operators

Almost all operators encountered in quantum mechanics are linear. A linear operator is any operator $\hat{A}$ satisfying the following two conditions:

$$\begin{aligned}\hat{A}(f+g)&=\hat{A}f+\hat{A}g,\\\hat{A}(cf)&=c\hat{A}f,\end{aligned} \tag{21.1.8}$$

where c is a constant and f and g are functions. As an example, consider the operators $\frac{d}{dx}$ and $()^2$. We can see that $\frac{d}{dx}$ is a linear operator because:

$$\begin{aligned} \frac{d}{dx}[f(x)+g(x)] &= \frac{d}{dx}f(x)+\frac{d}{dx}g(x), \\ \frac{d}{dx}[cf(x)] &= c(d/dx)f(x). \end{aligned} \tag{21.1.9}$$

However, $()^2$ is not a linear operator because:

$$(f(x)+g(x))^2 \neq (f(x))^2+(g(x))^2 \tag{21.1.10}$$

Hermitian Operators

Hermitian operators are characterized by the self-adjoint property:

$$\int \psi_a^*(\hat{A}\psi_a)d\mathbf{r} = \int \psi_a(\hat{A}\psi_a)^* d\mathbf{r}, \tag{21.1.11}$$

where the integral is performed over all space. This property guarantees that all the eigenvalues of the operators are real. Defining a as the eigenvalue of operator $\hat{A}$ using:

$$\hat{A}\psi(\mathbf{r}) = a\psi(\mathbf{r}), \tag{21.1.12}$$

we can prove that a is real by replacing Equation 21.1.12into Equation 21.1.11:

$$\begin{aligned} a\int \psi_a^*\psi_a d\mathbf{r} &= a^*\int \psi_a\psi_a^* d\mathbf{r} \\ (a-a^*)\int |\psi_a|^2 d\mathbf{r} &= 0, \end{aligned} \tag{21.1.13}$$

and since $|\psi_a|^2$ is never negative, either $a=a^*$ or $\psi_a=0$. Since $\psi_a=0$ is not an acceptable wavefunction, $a=a^*$, and a is real.

The following additional properties of Hermitian operators can also be proven with some work:

$$\int \psi^*\hat{A}\psi d\mathbf{r} = \int (\hat{A}\psi)^*\psi d\mathbf{r}, \tag{21.1.14}$$

and for any two states ψ_1 and ψ_2:

$$\int \psi_1^*\hat{A}\psi_2 d\mathbf{r} = \int (\hat{A}\psi_1)^*\psi_2 d\mathbf{r}. \tag{21.1.15}$$

Taking ψ_a and ψ_b as eigenfunctions of $\hat{A}$ with eigenvalues a and b with $a \neq b$, and using Equation 21.1.15, we obtain:

$$\begin{aligned} \int \psi_a^*\hat{A}\psi_b d\mathbf{r} &= \int (\hat{A}\psi_a)^*\psi_b d\mathbf{r} \\ b\int \psi_a^*\psi_b d\mathbf{r} &= a^*\int \psi_a^*\psi_b d\mathbf{r} \\ (b-a)\int \psi_a^*\psi_b d\mathbf{r} &= 0. \end{aligned} \tag{21.1.16}$$

Thus, since $a=a^*$, and since we assumed $b \neq a$, we must have $\int \psi_a^*\psi_b d\mathbf{r}=0$, i.e. ψ_a and ψ_b are orthogonal. In other words, eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal (or can be chosen to be so).

1. But they might not be strictly real.