Quantum Mechanics: Operators

Operators, eigenfunctions, eigenvalues

It turns out that operators are very important objects in quantum mechanics. In fact, all observable quantities, like position, momentum, angular momentum etc are represented by operators. So, first we will learn about operators and their properties.

Our basic definition of an operator is the following. *An operator is an object which acts on a function, and as a result gives another function.* Put mathematically, this statement says:

$$\hat{A}f(x) = g(x), \tag{1}$$

where $f(x)$ and $g(x)$ are two functions. One example is $\frac{d}{dx}$:

$$\frac{d}{dx}\sin(\alpha x) = \alpha\cos(\alpha x). \tag{2}$$

A *unit operator* may be represented by $\hat{1}$ which acts on any function, and yields the same function. For every operator, there can be a function such that the operator acts on the function and gives back the same function, times a number:

$$\hat{A}\psi(x) = a\psi(x). \tag{3}$$

In such a situation, this function is called the *eigenfunction* of that operator, and the number is its corresponding *eigenvalue*. A simple example involving a previously considered operator is

$$\frac{d}{dx}e^{i\alpha x} = i\alpha e^{i\alpha x}. \tag{4}$$

Here $e^{i\alpha x}$ is an eigenfunction of the operator $\frac{d}{dx}$, with $i\alpha$ as the eigenvalue. An operator can have more than one eigenfunction.

Commutation relations of operators

In general, two operators may *not commute*, which means that

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}. \tag{5}$$

If $\hat{A}\hat{B} = \hat{B}\hat{A}$, we say that the two operators *commute*. A convenient way to characterize the commutation property of two operators is by defining a *commutator* as follows

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{6}$$

Adjoint of an operator & Hermitian operators

For an operator $\hat{A}$, if there exist another operator $\hat{A}^\dagger$ such that

$$\int \psi^*(x)\hat{A}^\dagger\phi(x)dx = \left(\int \phi^*(x)\hat{A}\psi(x)dx\right)^* \tag{7}$$

for any $\psi(x), \phi(x)$, then $\hat{A}^\dagger$ is called the *adjoint* of $\hat{A}$. An operator is *Hermitian* if

$$\hat{A}^\dagger = \hat{A}. \tag{8}$$

Hermitian operators are of great importance in quantum mechanics. It is easy to show that **eigenvalues of a Hermitian operator are always real**. Let $\hat{B}$ be a Hermitian operator, and $\psi_b(x)$ is an eigenfunction of this operator, with an eigenvalue b. This implies $\hat{B}^\dagger = \hat{B}$ and $\hat{B}\psi_b(x) = b\psi_b(x)$. We write the definition of adjoint of $\hat{B}$, using the eigenfunction for both the functions:

$$\begin{aligned} \int \psi_b^*(x)\hat{B}\psi_b(x)dx &= \left(\int \psi_b^*(x)\hat{A}\psi_b(x)dx\right)^* \\ b\int \psi_b^*(x)\psi_b(x)dx &= b^*\int \psi_b^*(x)\psi_b(x)dx \\ b &= b^*, \end{aligned} \tag{9}$$

which means that the eigenvalue b is real.

Eqn. (7) can be written as

$$\int \psi^*(x)\hat{A}^\dagger\phi(x)dx = \int \phi(x)\left(\hat{A}\psi(x)\right)^* dx$$

Since the two entities on the RHS of the above, are functions, their order can be interchanged

$$\int \psi^*(x)\hat{A}^\dagger\phi(x)dx = \int \left(\hat{A}\psi(x)\right)^* \phi(x)dx.$$

Since the above is true for all $\phi(x)$, this implies

$$\left(\hat{A}\psi(x)\right)^* = \psi^*(x)\hat{A}^\dagger. \tag{10}$$

This relation should be remembered, as it will frequenctly come in useful.

If the adjoint of an operator is the same as the inverse of the operator, then the operator is said to be **unitary**. Thus a unitary operator is defined by

$$\hat{X}^\dagger = \hat{X}^{-1}.$$

This also implies $\hat{X}^\dagger\hat{X} = \hat{1}$. Unitary operators are also of great importance in quantum mechanics.

Operators in quantum mechanics

In quantum mechanics, all observable quantities are represented by operators. For describing an operator, one often needs a *representation*. So there may be more than one way of representing an operator. We will come back to this point later. For now, the only two operators in quantum mechanics that we have learnt till now, are position and momentum operators. They can be written in the *position representation* as follows:

$$\hat{x} = x, \qquad \hat{p} = -i\hbar\frac{d}{dx}. \tag{11}$$

Let us look at the commutation relation of these two operators. Commution relation can be found by letting the commutator act on an *arbitrary* function of x:

$$\begin{aligned} [\hat{x},\hat{p}]f(x) &= (\hat{x}\hat{p} - \hat{p}\hat{x})f(x) \\ &= x(-i\hbar\frac{d}{dx})f(x) - (-i\hbar\frac{d}{dx})xf(x) \\ &= -i\hbar xf'(x) + i\hbar f(x) + i\hbar xf'(x) \\ &= i\hbar f(x). \end{aligned} \tag{12}$$

Since the above is true for any arbitrary $f(x)$, we can write

$$[\hat{x}, \hat{p}] = i\hbar. \tag{13}$$

This is a very important commutation relation in quantum mechanics.

Eigenvalues hold an important place in quantum mechanics. They correspond to the *measured values* of the operator. One may represent an observable by a quantum operator, but when we measured a quantity, say momentum, we always get a number. So, it is only logical that there should be a number associated with a measured value of the observable.

Hamiltonion: The operator for energy

Now we can write the operator for the energy for a particle of mass m, experiencing a potential, simply by taking the classical expression for the energy, and replacing the momentum and position by their respective operators. The *Hamiltonian*, the operator for energy, is then given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}), \tag{14}$$

where the first term represents the kinetic energy, and the second term the potential energy. Since $\hat{x}$ and $\hat{p}$ are Hermitian operators, one can verify that $\hat{H}$ is also Hermitian, which implies that its eigenvalues will be real. It better be so, because the measured value of energy of any particle is real. The energy of the particle can be found out by solving the *eigenvalue equation*

$$\hat{H}\psi(x) = E\psi(x),$$

which, when expanded, looks like

$$\boxed{\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\psi(x) = E\psi(x)}, \tag{15}$$

where $\psi(x)$ is the eigenfunction of the Hamiltonian, and E is the corresponding eigenvalue. This equation is also referred to as the *time-independent Schrödinger equation*. It may be contrasted with the time-*dependent* Schrödinger equation that we wrote down earlier:

$$\boxed{i\hbar\frac{\partial\psi(x)}{\partial t} = \left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\psi(x)}. \tag{16}$$

In quantum mechanics, understanding a system generally means find the eigenfunctions and eigenvalues of the Hamiltonian. One can represent the time-dependent Schrödinger equation more compactly as

$$i\hbar\frac{\partial\psi(x)}{\partial t} = \hat{H}\psi(x).$$