3.5: Operators

An operator, O (say), is a mathematical entity that transforms one function into another: that is,

$$O(f(x)) \rightarrow g(x). \tag{3.5.1}$$

For instance, x is an operator, because $x\,f(x)$ is a different function to $f(x)$, and is fully specified once $f(x)$ is given. Furthermore, d/dx is also an operator, because $df(x)/dx$ is a different function to $f(x)$, and is fully specified once $f(x)$ is given. Now,

$$x\,\frac{df}{dx} \neq \frac{d}{dx}(x\,f)\,. \tag{3.5.2}$$

This can also be written

$$x\,\frac{d}{dx} \neq \frac{d}{dx}\,x, \tag{3.5.3}$$

where the operators are assumed to act on everything to their right, and a final $f(x)$ is understood [where $f(x)$ is a general function]. The previous expression illustrates an important point. Namely, in general, operators do not commute with one another. Of course, some operators do commute. For instance,

$$x\,x^{\,2} = x^{\,2}\,x. \tag{3.5.4}$$

Finally, an operator, O, is termed linear if

$$O(c\,f(x)) = c\,O(f(x)), \tag{3.5.5}$$

where f is a general function, and c a general complex number. All of the operators employed in quantum mechanics are linear.

Now, from Equations ([e3.22]) and ([e3.38]),

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi^{\ast}\,x\,\psi\,dx,$$

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi^{\ast}\left(-{\rm i}\,\hbar\,\frac{\partial}{\partial x}\right)\psi\,dx.$$

These expressions suggest a number of things. First, classical dynamical variables, such as x and p, are represented in quantum mechanics by linear operators that act on the wavefunction. Second, displacement is represented by the algebraic operator x, and momentum by the differential operator $-{\rm i}\,\hbar\,\partial/\partial x$: that is, \[\label{e3.54} p \equiv -{\rm i}\,\hbar\,\frac{\partial}{\partial x}.\]

Finally, the expectation value of some dynamical variable represented by the operator $O(x)$ is simply

$$\langle O\rangle = \int_{-\infty}^{\infty}\psi^{\ast}(x,t)\,O(x)\,\psi(x,t)\,dx. \tag{3.5.6}$$

Clearly, if an operator is to represent a dynamical variable that has physical significance then its expectation value must be real. In other words, if the operator O represents a physical variable then we require that $\langle O\rangle = \langle O\rangle^{\ast}$, or

$$\int_{-\infty}^{\infty}\psi^{\ast}\,(O\,\psi)\,dx = \int_{-\infty}^{\infty}(O\,\psi)^{\ast}\,\psi\,dx, \tag{3.5.7}$$

where $O^{\ast}$ is the complex conjugate of O. An operator that satisfies the previous constraint is called an *Hermitian* operator. It is easily demonstrated that x and p are both Hermitian. The *Hermitian conjugate*, $O^{\dagger}$, of a general operator, O, is defined as follows:

$$\int_{-\infty}^{\infty}\psi^{\ast}\,(O\,\psi)\,dx = \int_{-\infty}^{\infty}(O^{\dagger}\,\psi)^{\ast}\,\psi\,dx. \tag{3.5.8}$$

The Hermitian conjugate of an Hermitian operator is the same as the operator itself: that is, $p^{\dagger} = p$. For a non-Hermitian operator, O (say), it is easily demonstrated that $(O^{\dagger})^{\dagger} = O$, and that the operator $O + O^{\dagger}$ is Hermitian. Finally, if A and B are two operators, then $(A\,B)^{\dagger} = B^{\dagger}\,A^{\dagger}$.

Suppose that we wish to find the operator that corresponds to the classical dynamical variable $x\,p$. In classical mechanics, there is no difference between $x\,p$ and $p\,x$. However, in quantum mechanics, we have already seen that $x\,p \neq p\,x$. So, should we choose

$x\,p$ or $p\,x$? Actually, neither of these combinations is Hermitian. However, $(1/2)\,[x\,p+(x\,p)^\dagger]$ is Hermitian. Moreover, $(1/2)\,[x\,p+(x\,p)^\dagger]=(1/2)\,(x\,p+p^\dagger\,x^\dagger)=(1/2)\,(x\,p+p\,x)$, which neatly resolves our problem of the order in which to place x and p.

It is a reasonable guess that the operator corresponding to energy (which is called the Hamiltonian, and conventionally denoted H) takes the form

$$H\equiv\frac{p^{\,2}}{2\,m}+V(x). \tag{3.5.9}$$

Note that H is Hermitian. Now, it follows from Equation ([e3.54]) that

$$H\equiv-\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}}{\partial x^{\,2}}+V(x). \tag{3.5.10}$$

However, according to Schrödinger's equation, ([e3.1]), we have

$$-\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}}{\partial x^{\,2}}+V(x)={\rm i}\,\hbar\,\frac{\partial}{\partial t}, \tag{3.5.11}$$

so

$$H\equiv{\rm i}\,\hbar\,\frac{\partial}{\partial t}. \tag{3.5.12}$$

Thus, the time-dependent Schrödinger equation can be written

$${\rm i}\,\hbar\,\frac{\partial\psi}{\partial t}=H\,\psi. \tag{3.5.13}$$

Finally, if $O(x,p,E)$ is a classical dynamical variable that is a function of displacement, momentum, and energy then a reasonable guess for the corresponding operator in quantum mechanics is $(1/2)\,[O(x,p,H)+O^\dagger(x,p,H)]$, where $p=-{\rm i}\,\hbar\,\partial/\partial x$, and $H={\rm i}\,\hbar\,\partial/\partial t$.

Contributors and Attributions

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