Operators

Physical properties		Operators	
Name of Operator	Observables	Operators	Symbols
Position	Position with x coordinate	x	x
Momentum	x component of momentum	-iħ . ∂/∂x	p_x
Angular momentum	z component of angular momentum	-iħ . ∂/∂Φ	L_z
K.E operator	Kinetic energy	$-ħ^2/2m$. ∂/∂x	T
P.E operator	Potential energy	$V_{(x)}$	V
Total energy (E)	Hamiltonian operator (Time-Independent)	$-ħ^2/2m.∂/∂x$ + V(x)	Ĥ
Total energy (E)	Hamiltonian operator (Time-dependent)	-iħ . ∂/∂t	Ĥ

Addition and Subtraction of Operators

$$(\hat{A}+\hat{B})f(x)=\hat{A}f(x)+\hat{B}f(x)$$
$$(\hat{A}-\hat{B})f(x)=\hat{A}f(x)-\hat{B}f(x)$$

Products of Operators

$$\hat{A}\hat{B}f(x)=\hat{A}\{\hat{B}f(x)\}$$

In general, $\hat{A}\hat{B}f(x)\neq\hat{B}\hat{A}f(x)$

Let us consider, $\hat{A}=x\ and\ \hat{B}=\frac{\mathrm{d}}{\mathrm{d}x}$

$$f(x)=3x^2$$

$$(\hat{A}+\hat{B})f(x)=\left(x+\frac{d}{dx}\right)3x^2$$
$$=x\times 3x^2+\frac{\mathrm{d}}{\mathrm{d}x}(3x^2)$$
$$=3x^3+6x$$

$$\hat{A}\hat{B}f(x)=x\times\frac{\mathrm{d}}{\mathrm{d}x}3x^2=x\times 6x=6x^2$$
$$\hat{B}\hat{A}f(x)=\frac{\mathrm{d}}{\mathrm{d}x}(x\times 3x^2)=\frac{\mathrm{d}}{\mathrm{d}x}3x^3=9x^2$$

Commutators

If two operators commute then,

$$\hat{A}\hat{B}f(x) = \hat{B}\hat{A}f(x)$$

$$[\hat{A}\hat{B}]f(x) = (\hat{A}\hat{B} - \hat{B}\hat{A})f(x) = 0$$

Commutator, $[\hat{A}\hat{B}] = (\hat{A}\hat{B} - \hat{B}\hat{A})$

In the previous example,

$$\hat{A}\hat{B}f(x) = x \times \frac{\mathrm{d}}{\mathrm{d}x}3x^2 = x \times 6x = 6x^2$$

$$\hat{B}\hat{A}f(x) = \frac{\mathrm{d}}{\mathrm{d}x}(x \times 3x^2) = \frac{\mathrm{d}}{\mathrm{d}x}3x^3 = 9x^2$$

$$[\hat{A}\hat{B}]f(x) = (\hat{A}\hat{B} - \hat{B}\hat{A})f(x) = 6x^2 - 9x^2 = 3x^2 = f(x)$$

$$\Rightarrow [\hat{A}\hat{B}]f(x) = f(x)$$

$$\Rightarrow [\hat{A}\hat{B}] = 1$$

Example 3.1. Find the commutators of each of the following pairs of operators

(*a*) $\frac{d^2}{dx^2}, x\frac{d}{dx}$ (*b*) $x^3, \frac{d}{dx}$

(*a*) $$\left[\frac{d^2}{dx^2}, x\frac{d}{dx}\right] f(x) = \frac{d^2}{dx^2}\left(x\frac{d}{dx}\right) f(x) - \left(x\frac{d}{dx}\right)\left(\frac{d^2}{dx^2}\right) f(x)$$

$$= \frac{d}{dx}\left(\frac{d}{dx} + x\frac{d^2}{dx^2}\right) f(x) - x\frac{d}{dx}\left(\frac{d^2}{dx^2}\right) f(x)$$

$$= \left(\frac{d^2}{dx^2} + \frac{d^2}{dx^2} + 2x\frac{d^3}{dx^3}\right) f(x) - x\frac{d^3}{dx^3} f(x) - x\frac{d^3}{dx^3} f(x)$$

$$= 2\frac{d^2}{dx^2} f(x);\ \text{since}\ \left[\frac{d}{dx}\left(\frac{d^2}{dx^2}\right) f(x) = 2\frac{d^3}{dx^3} f(x)\right]$$

Deleting the arbitrary function $f(x)$, we find

$$\left[\frac{d^2}{dx^2}, x\frac{d}{dx}\right] = 2\frac{d^2}{dx^2}$$

(*b*) $$\left[x^3, \frac{d}{dx}\right] f(x) = \left[x^3\left(\frac{d}{dx}\right) - \left(\frac{d}{dx}\right) x^3\right] f(x)$$

$$= x^3\frac{d}{dx} f(x) - \frac{d}{dx}[x^3 f(x)]$$

$$= x^3\frac{d}{dx} f(x) - 3x^2 f(x) - x^3\frac{d}{dx} f(x)$$

$$= -3x^2 f(x)$$

Deleting the arbitrary functions $f(x)$ we get the operator equation

$$\left[x^3, \frac{d}{dx}\right] = -3x^2$$

Linear Operators

1.For the functions being added or subtracted, the function can be applied to all functions individually.

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

2.Constants are not affected by the application of linear operators.

$\hat{A}\,\{cf(x)\} = c\hat{A}f(x)$

Example: $$\frac{\mathrm{d}}{\mathrm{d}x}(3x^2 + 6x) = 6x + 6$$

Hermitian Operators

1.A hermitian operator can be flipped over to the other side. In other words, it justifies the complex conjugate transpose of matrices.

If Â is hermitian, {g|Â .f} = {f|Â .g}

2.The eigenvalues of a hermitian operator are always real.

from above example, {f|Â .f} must be a real value.

3.The eigenvalues are orthonormal by convention for a hermitian operator. in other words, they have a complete set of orthonormal eigenfunctions (eigenvectors).

Example:

$\Psi_1 = e^{-ix}$

$\Psi_2 = \cos x$

$$\hat{A} = \frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

$$\int \cos x \frac{d^2}{dx^2}\left(\mathrm{e}^{-\mathrm{i}k}\right) \mathrm{d}x = -\mathrm{i} \int \cos x \frac{\mathrm{d}}{\mathrm{d}x}\left(e^{-ix}\right) \mathrm{d}x = -\int \cos x e^{-ix}\, dx$$

$$\int \frac{\mathrm{d}^2}{\mathrm{d}x^2} \cos x \mathrm{e}^{-\mathrm{i}x}\, \mathrm{d}x = -\int \frac{\mathrm{d}}{\mathrm{d}x^2} \sin x \mathrm{e}^{-\mathrm{i}x}\, \mathrm{d}x = -\int \cos x^{e^{-ix}}\, dx$$

Eigen functions and eigen values

If for an operator $\hat{A}$, we can write

$\hat{A}f = kf$ Where k is a constant

then, **f is called an eigen function of $\hat{A}$** and **k is called its eigen value.**

Example: e^{ikx} is an eigenfunction of a operator $\hat{P}_x = -ih\frac{\partial}{\partial x}$

$F(x) = e^{ikx}$

$= -i\,h\frac{\partial}{\partial x}e^{ikx}$

$= -i^2\,hk^2e^{ikx}$

$= h\,k^2e^{ikx}$ Thus e^{ikx} is an eigenfunction

Expectation values

When a system is in an *eigenstate* of observable $\hat{A}$ (i.e., when the wavefunction is an eigenfunction of the operator) then the expectation value of $\hat{A}$ is the eigenvalue of the wavefunction. Thus if

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

Average Value, $\langle A \rangle$

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

$$= \int \psi^*(\mathbf{r})a\psi(\mathbf{r})d\mathbf{r}$$

$$= a\int \psi^*(\mathbf{r})\psi(\mathbf{r})d\mathbf{r}$$

$$= a$$