Schrödinger Equation

Operator in QM

Dr Mohammad Abdur Rashid

de Broglie wave for a particle

The wave function or de Broglie wave for a free particle with momentum p and energy E is given by

$$\Psi(x,t) = e^{i(px-Et)/\hbar}$$

Since the wave function contains all the information about the system, it is often of interest to find appropriate operators to extract information from the wave function.

Momentum operator $\hat{p}$

We take

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) = \frac{\hbar}{i}\frac{\partial}{\partial x}e^{i(px-Et)/\hbar}$$
$$= \frac{\hbar}{i}\frac{ip}{\hbar}e^{i(px-Et)/\hbar}$$
$$= p\Psi(x,t)$$

where the p factor is just the momentum.

Momentum operator $\hat{p}$

We thus identify the **momentum operator** $\hat{p}$ as

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

and we have verified that acting on the wave function $\Psi(x,t)$ for a particle of momentum p it gives p times the wave function:

$$\hat{p}\Psi(x,t) = -i\hbar\frac{\partial}{\partial x}\Psi(x,t) = p\Psi(x,t).$$

Momentum operator $\hat{p}$

The momentum operator acts on wave functions, which are functions of space and time to give another function of space and time. Since $\hat{p}$ acting on $\Psi(x,t)$ gives a number (p, in fact) times $\Psi(x,t)$ we say that $\Psi(x,t)$ is an **eigenstate** of $\hat{p}$. We also say that $\Psi(x,t)$ is a state of **definite momentum**.

Energy operator $\hat{E}$

Let us now consider extracting the energy information from the free particle wave function. This time we must avail ourselves of the time derivative:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Psi(x,t) &= i\hbar\frac{\partial}{\partial t}e^{i(px-Et)/\hbar} \\
&= i\hbar\,\frac{-iE}{\hbar}\,e^{i(px-Et)/\hbar)} \\
&= E\Psi(x,t).
\end{aligned}
$$

Energy operator $\hat{E}$

Hence we define the total energy operator $\hat{E}$ such that

$$\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}.}$$

$$\boxed{\hat{E}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) = E\Psi(x,t)}$$

Eigenvalue Equation

$$\hat{p}\Psi(x,t) = p\Psi(x,t), \qquad \hat{E}\Psi(x,t) = E\Psi(x,t)$$

(Operator)(function)=(constant factor)×(same function)

(Operator)(eigenfunction)=(eigenvalue)×(eigenfunction)

Eigenvalue equation: $\hat{\Omega}\Psi = \omega\Psi$

Eigenvalue Equation

Example: Show that e^{ax} is an eigenfunction of the operator $\mathrm{d}/\mathrm{d}x$, and find the corresponding eigenvalue. Show that e^{ax^2} is not an eigenfunction of $\mathrm{d}/\mathrm{d}x$.

We need to operate on the function with the operator and check whether the result is a constant factor times the original function.

Eigenvalue Equation

For $\hat{\Omega} = \frac{\mathrm{d}}{\mathrm{d}x}$ and $\Psi = e^{ax}$:

$$\hat{\Omega}\Psi = \frac{\mathrm{d}}{\mathrm{d}x}e^{ax} = ae^{ax} = a\Psi$$

Therefore e^{ax} is indeed an eigenfunction of $\frac{\mathrm{d}}{\mathrm{d}x}$, and its eigenvalue is a.

Eigenvalue Equation

For $\hat{\Omega} = \frac{\mathrm{d}}{\mathrm{d}x}$ and $\Psi = e^{ax^2}$:

$$\hat{\Omega}\Psi = \frac{\mathrm{d}}{\mathrm{d}x} e^{ax^2} = 2axe^{ax} = 2ax\Psi$$

which is not an eigenvalue equation of $\hat{\Omega}$. Even though the same function Ψ occurs on the right-hand side.

Energy operator $\hat{E}$

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

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

For a free particle the total energy is the kinetic energy and is given in terms of momentum such that

$$E = \frac{p^2}{2m}.$$

Energy operator $\hat{E}$

We write

$$E\Psi = \frac{p^2}{2m}\Psi = \frac{p}{2m}\,p\Psi = \frac{p}{2m}\,\hat{p}\Psi$$

$$= \frac{p}{2m}\,(-i\hbar)\frac{\partial}{\partial x}\Psi$$

Since p is a constant we can move the p factor on the last right-hand side close to the wave function and then replace it by the momentum operator.

Energy operator $\hat{E}$

$$
\begin{aligned}
E\Psi &= \frac{1}{2m}(-i\hbar)\frac{\partial}{\partial x}p\Psi \\
&= \frac{1}{2m}(-i\hbar)\frac{\partial}{\partial x}(-i\hbar)\frac{\partial}{\partial x}\Psi \\
&= -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}.
\end{aligned}
$$

$$\hat{E} \equiv \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

Energy operator $\hat{E}$

For the free particle wave function $\Psi(x,t) = e^{i(px-Et)/\hbar}$ we show that

$$\begin{aligned} \hat{E}\Psi(x,t) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{i(px-Et)/\hbar} \\ &= -\frac{\hbar^2}{2m}\left(\frac{ip}{\hbar}\right)^2 e^{i(px-Et)/\hbar} \\ &= \frac{p2}{2m}\Psi(x,t) \\ &= E\Psi(x,t) \end{aligned}$$

Free particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = E\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi$$

For a free particle the de Broglie wave function satisfies the differential equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

The free-particle Schrödinger equation.

$$\Psi = e^{i(px-Et)/\hbar}$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

$$\hat{E} \equiv \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Kinetic energy operator

Using the energy operator the free-particle Schrödinger equation can be written as:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{E}\Psi(x,t).$$

The kinetic energy operator: $$\hat{T} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Hamiltonian operator

If the particle is not free but rather is moving in some external potential $V(x,t)$, the total energy of the particle is the sum of kinetic and potential energies:

$$E = \frac{p^2}{2m} + V(x,t).$$

This suggests that the total energy operator should be:

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t).$$

Hamiltonian operator

In case of a particle in a potential $V(x,t)$ the Schrödinger equation is written as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\Psi(x,t).$$

The energy operator $\hat{E}$ is usually called the Hamiltonian operator $\hat{H}$, so one has

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

The Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$$

For a particle quantum mechanical of mass m moving in a potential $V(x,t)$ the Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

Position operator

We introduce another very important operator: the **position operator** $\hat{x}$ that acting on functions of x gives another function of x as follows:

$$\boxed{\hat{x} f(x) \equiv x f(x).}$$

$$\boxed{\hat{x}^k f(x) \equiv x^k f(x)}$$

Schrödinger equation and wave function

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$$

The Schrödinger equation has an explicit i on the left-hand side. This i shows that it is impossible to find a solution for real Ψ. If Ψ were real the right-hand side of the equation would be real but the left-hand side would be imaginary. Thus, the Schrödinger equation forces us to work with complex wave functions.

The Schrödinger equation in 3D

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right)\Psi(\mathbf{r},t)}$$

The Laplacian operator: $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$

Operators in 3D

$$\hat{\mathbf{r}} \equiv (\hat{x}, \hat{y}, \hat{z})$$

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)$$

$$\hat{\mathbf{p}} \equiv -i\hbar\nabla$$

$$\nabla \equiv (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$$

$$\hat{T} \equiv -\frac{\hbar^2}{2m}\nabla^2$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Thank You

To receive notification of new video please subscribe to our channel.

You may also let us know your comments.