Schrödinger Equation

Operator in QM

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Schrödinger Equation

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

Time dependent SE

$$\boxed{\hat{H}\Psi(x) = E\Psi(x)}$$

Time independent SE

$\hat{H}$ is called hamiltonian operator.

Schrödinger Equation

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

Time
dependent
SE

An operator is a mathematical rule that carries out a mathematical operation on a function.

Schrödinger Equation

In one dimension for a particle moving in a potential $V(x)$ the hamiltonian operator $\hat{H}$ is written as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

Eigenvalue Equation

$$\boxed{\hat{H}\Psi(x) = E\Psi(x)}$$

Time independent SE

$$(\text{Operator})(\text{function}) = (\text{constant factor}) \times (\text{same function})$$

Eigenvalue equation

$$\hat{\Omega}\psi = \omega\psi$$

Eigenvalue Equation

$$\begin{aligned}&(\text{Operator})(\text{eigenfunction})\\&\qquad=(\text{eigenvalue})\times(\text{eigenfunction})\end{aligned}$$

Show that e^{ax} is an eigenfunction of the operator d/dx, and find the corresponding eigenvalue. Show that e^{ax^2} is not an eigenfunction of d/dx.

Eigenvalue Equation

Answer For $\hat{\Omega} =$ d/dx (the operation 'differentiate with respect to x') and $\psi = \mathrm{e}^{ax}$:

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

Eigenvalue Equation

For $\psi = \mathrm{e}^{ax^2}$,

$$\hat{\Omega}\psi = \frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{ax^2} = 2ax\mathrm{e}^{ax^2} = 2ax \times \psi$$

which is not an eigenvalue equation of $\hat{\Omega}$. Even though the same function ψ occurs on the right, ψ is now multiplied by a variable factor ($2ax$), not a constant factor. Alternatively, if the right hand side is written $2a(x\mathrm{e}^{ax^2})$, we see that it is a constant ($2a$) times a *different* function.

Eigenvalue Equation

$$\boxed{\hat{H}\Psi(x) = E\Psi(x)}$$

Time independent SE

$$(\text{Operator corresponding to an observable})\psi$$
$$= (\text{value of observable}) \times \psi$$

Operator in QM

$$(\text{Operator corresponding to an observable})\psi = (\text{value of observable}) \times \psi$$

$$\hat{x} = x \times \qquad \hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$$

position and momentum operators

Operator in QM

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

$$\begin{aligned}
\hat{p}_x\Psi(x,t) &= A\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}e^{-i(Et-xp_x)/\hbar} \\
&= A\frac{\hbar}{i}e^{-i(Et-xp_x)/\hbar}[-i(-p_x)/\hbar] \\
&= Ap_x e^{-i(Et-xp_x)/\hbar} \\
&= p_x\Psi(x,t)
\end{aligned}$$

Operator in QM

To get the kinetic energy operator, we make use of the classical relation between kinetic energy and linear momentum, which in one dimension is

$$E_{\mathrm{k}} = p_x^2 / 2m$$

$$\hat{E}_{\mathrm{k}} = \frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\right) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

Schrödinger Equation

In one dimension for a particle moving in a potential $V(x)$ the hamiltonian operator $\hat{H}$ is written as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

Operator in QM

Position x	x
Potential Energy $V(x)$	$V(x)$
Momentum p_x	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
Kinetic Energy $\frac{p_x^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

Operator in QM

Total Energy (Kinetic + Potential) E_{Total}	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
Total Energy (Time Version) E_{Total}	$-\frac{\hbar}{i}\frac{\partial}{\partial t}$

Schrödinger Equation

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

Time dependent SE

Operator in QM

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

$$\begin{aligned}
\hat{E}\Psi(x,t) &= Ai\hbar\frac{\mathrm{d}}{\mathrm{d}t}e^{-i(Et-xp_x)/\hbar} \\
&= Ai\hbar e^{-i(Et-xp_x)/\hbar}[-iE/\hbar] \\
&= AEe^{-i(Et-xp_x)/\hbar} \\
&= E\Psi(x,t)
\end{aligned}$$

Operator in QM

Every observable in quantum mechanics is represented by a linear, hermitian operator

A linear operator is one which satisfies the identity $\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$

Operator in QM

In any measurement of an observable A, associated with an operator $\hat{A}$, the only possible results are the eigenvalues a_n, which satisfy an eigenvalue equation

$$\hat{A}\psi_n = a_n\psi_n$$

Schrödinger Equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x)$$

One dimensional time-independent Schrödinger Equation

Schrödinger Equation

$$\left[-\frac{\hbar^2}{2m}\left\{\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{\mathrm{d}^2}{\mathrm{d}z^2}\right\}+V(x,y,z)\right]\Psi(x,y,z)$$
$$=E\Psi(x,y,z)$$

Three dimensional time-independent Schrödinger Equation

Schrödinger Equation

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

One dimensional time-dependent Schrödinger Equation

Thank You

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