

Ground rules



<https://slideplayer.com/slide/5291168/>

Time dependent Schrodinger Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x, y, z, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \Psi(x, y, z, t)$$

$$\text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Classical wave equation for de Broglie waves

Separation of variables:

$$\Psi_n(x, y, z, t) = \psi_n(x, y, z) \phi(t)$$

Separation of variables

$$i\hbar \frac{\partial}{\partial t} \psi_n(x, y, z) \phi(t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \psi_n(x, y, z) \phi(t)$$

$$\psi_n(x, y, z) \cdot i\hbar \frac{\partial \phi(t)}{\partial t} = \phi(t) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_n(x, y, z) + V(x, y, z) \cdot \psi_n(x, y, z) \right]$$

$$\frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \left[-\frac{\hbar^2}{2m \cdot \psi_n(x, y, z)} \nabla^2 \psi_n(x, y, z) + V(x, y, z) \cdot \psi_n(x, y, z) \right] = W$$

Separation constant

$$\Psi_n(x, y, z, t) = \psi_n(x, y, z) \phi(t)$$

Separation of variables

$$i\hbar \frac{\partial}{\partial t} \psi_n(x, y, z) \phi(t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \psi_n(x, y, z) \phi(t)$$

\hat{H} , Hamiltonian operator

$$\psi_n(x, y, z) \cdot i\hbar \frac{\partial \phi(t)}{\partial t} = \phi(t) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_n(x, y, z) + V(x, y, z) \cdot \psi_n(x, y, z) \right]$$

$$\frac{i\hbar}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \left[-\frac{\hbar^2}{2m \cdot \psi_n(x, y, z)} \nabla^2 \psi_n(x, y, z) + V(x, y, z) \cdot \psi_n(x, y, z) \right] = W$$

$$\boxed{\phi(t)} \frac{i\hbar}{\partial t} = W; \quad \left[-\frac{\hbar^2}{2m \cdot \psi_n(x, y, z)} \nabla^2 \psi_n(x, y, z) + V(x, y, z) \cdot \psi_n(x, y, z) \right] = W$$

$e^{-iWt/\hbar}$

$$\Psi_n(x, y, z, t) = \psi_n(x, y, z) e^{-iWt/\hbar}$$

Stationary states

In classical mechanics \hat{H} represents total energy

We can therefore write

$$\hat{H}\psi = W\psi \quad \text{as} \quad \hat{H}\psi = E\psi$$

$$\Psi_n(x, y, z, t) = \psi_n(x, y, z)e^{-iE_nt/\hbar}$$

Each $\psi_n(x, y, z)$: a particular value of energy E_n

☞ a particular **Energy eigenstate (Stationary state)**

Quantization? Not yet!!

Eigenvalues and Eigenfunctions

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Schrodinger equation is an eigenvalue equation

There can be many solutions $\psi_n(\mathbf{x})$ each corresponding to different energy E_n

Laws of Quantum Mechanics

Mathematical description of Quantum mechanics: built upon the concept of operators

Classical Variable

Position, x

Momentum, $p_x = mv$

Kinetic Energy, $T_x = \frac{p_x^2}{2m}$

Kinetic Energy, $T = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$

Potential Energy, $V(x)$

QM Operator

\hat{x}

$\hat{p}_x = \frac{\hbar}{i} \frac{d}{dx} = -i\hbar \frac{d}{dx}$

$\hat{T}_x = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$

$\hat{T} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$

$\hat{V}(x)$

Laws of Quantum Mechanics

The values which come up as result of an experiment are the eigenvalues of the appropriate operator

In any measurement of observable associated with operator \hat{A} , the only values that will be ever observed are the eigenvalues a_n , which satisfy the eigenvalue equation:

$$\hat{A} \cdot \Psi_n = a_n \cdot \Psi_n$$

Ψ_n are the eigenfunctions of the system and a_n are corresponding eigenvalues

If the system is in state Ψ_k , a measurement on the system will yield an eigenvalue a_k

Laws of Quantum Mechanics

Only real eigenvalues will be observed, which will specify a number corresponding to the classical variable

$$\text{If } Y(x) = \sin(cx)$$

$$\frac{d}{dx} Y(x) = c \times \cos(cx)$$

$$\frac{d^2}{dx^2} Y(x) = -c^2 \times \sin(cx) = -c^2 \times Y(x)$$

$$\text{If } Y(x) = e^{ax}$$

$$\frac{d}{dx} Y(x) = a \times e^{ax}$$

$$\frac{d^2}{dx^2} Y(x) = a^2 \times e^{ax} = a^2 \times Y(x)$$

There may be, and typically are, many eigenfunctions for the same QM operator!

Laws of Quantum Mechanics

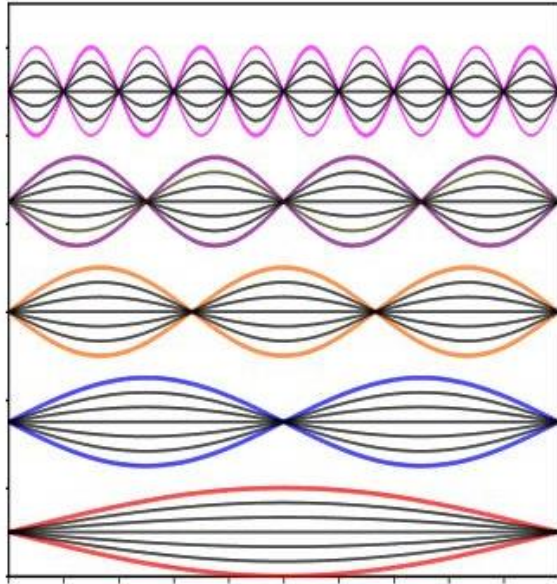
All the eigenfunctions of Quantum Mechanical operators are “Orthogonal”

$$\int_{-\infty}^{+\infty} \psi_m^*(x) \psi_n(x) dx = \langle \psi_m | \psi_n \rangle = 0 \quad \text{for } m \neq n$$

Superposition of states

Schrodinger equation: Classical wave equation for de Broglie waves

General solutions of Classical wave equation: **Standing waves**



Superposition of **Normal modes**
(Length: Half integral multiple of wavelength)

Solutions of Schrodinger equation:
Linear combination of wavefunctions that are
orthogonal to each other

Before and after measurement

Measurement: Property has a value of P

Before measurement:

Realist: Value = P (Einstein)

⇒ *Quantum theory is incomplete*

Orthodox: Entanglement (Bohr,
Copenhagen interpretation)

⇒ *Measurement produces the value*

Agnostic: Don't know, don't care

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Immediately after measurement:

Same Value = P



Wavefunction collapse

But what is this wavefunction?



Google Doodle, December 11, 2017