Learning Objectives

1. Revision

2. Schrodinger's equation

3. What is quantum mechanics?

References: 1) Quantum Physics by H.C. Verma

Introduction to Quantum Mechanics - David J. Griffiths

Atomic structure: Bohr's model-shortcomings

1) uncertainty principle, 2) dual behaviour of particle

concepts of quantum mechanics

- **Quantum mechanics** is a science that deals with the study of the motions of the microscopic objects that have both observable wave like and particle like properties.
- It specifies the laws of motion that these objects obey.
- *When quantum mechanics is applied to macroscopic objects (for which wave-like properties are insignificant) the results are the same as those from the classical mechanics.*

Schrödinger's equation

Newton's law - basic law of dynamics for classical physics.
"STATE" of the particle at any instant is described in classical physics by giving its position and velocity at that instant. If these quantities are known at $t=0$, we can predict their values at any later time by solving following equation.

$$m\frac{d^2x}{dt^2} = F(x,t)$$

← force on the particle when it is at position x and time t.

In Quantum mechanics, basic equation governing dynamics of a particle is called Schrödinger's equation.

$$H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$$

Hamiltonian operator
(operator corresponding to total energy of the system)

Two new terms

1. Wavefunction-> Accepted Wavefunction->

Operators->Measurable quantity-> Eigenvalue and Eigenfunction

2. Hamiltonian

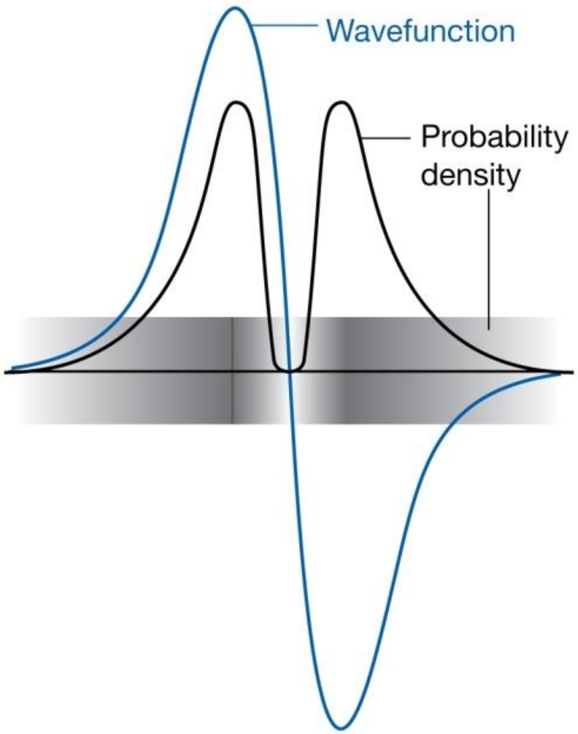
Well behaved wavefunction

1) ψ must be continuous and single valued everywhere.

2) $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must be continuous and single valued everywhere.

3) ψ must be normalizable, which means that ψ must go to 0 as $x \to \pm\infty$, $y \to \pm\infty$, $z \to \pm\infty$ in order that $\int |\psi|^2 dV$ over all space be a finite constant.

$$\int_{all\_space} \Psi^* \Psi \, d\tau = 1$$



Wavefunction: Acceptable or Not

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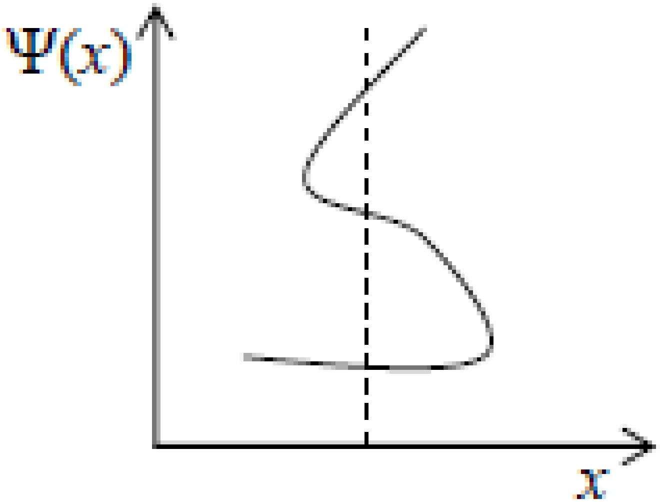

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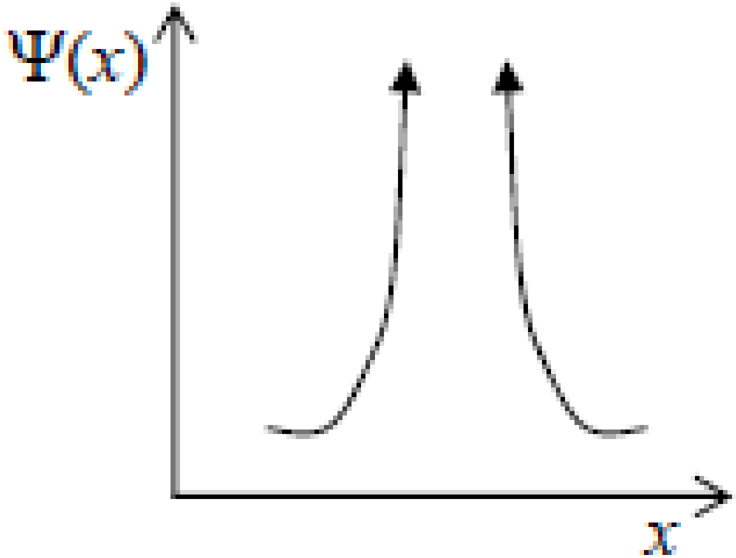

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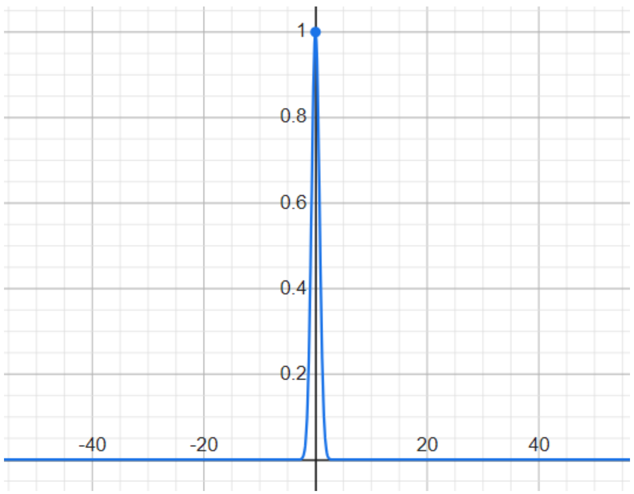

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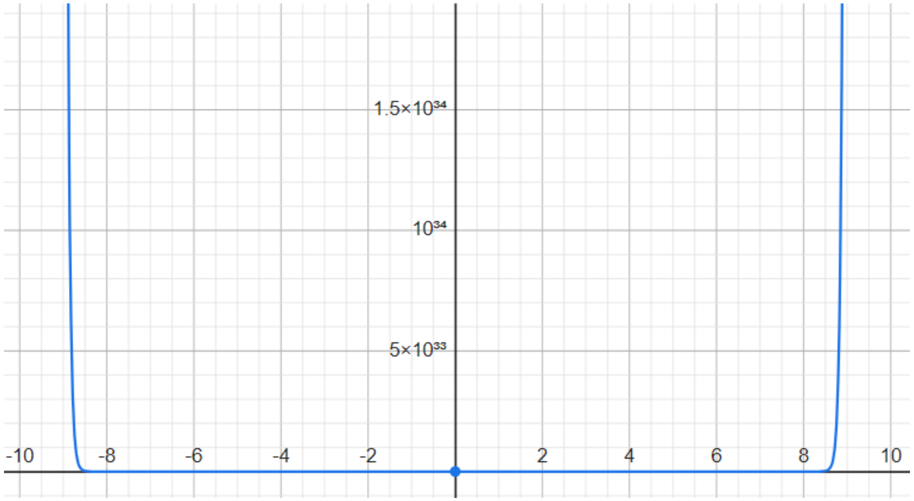

Wavefunction: Acceptable or Not

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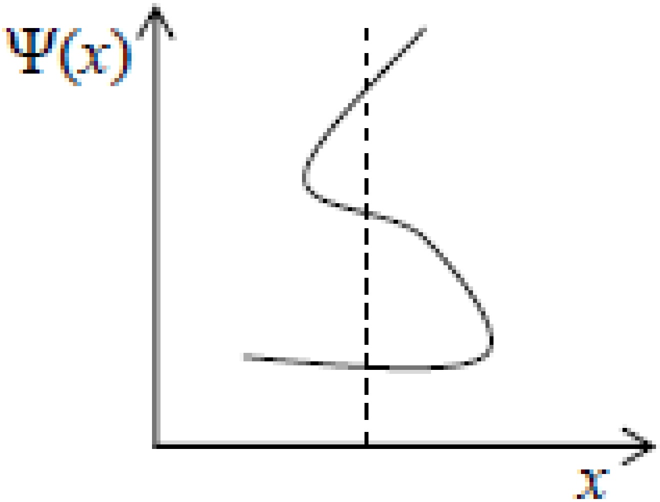

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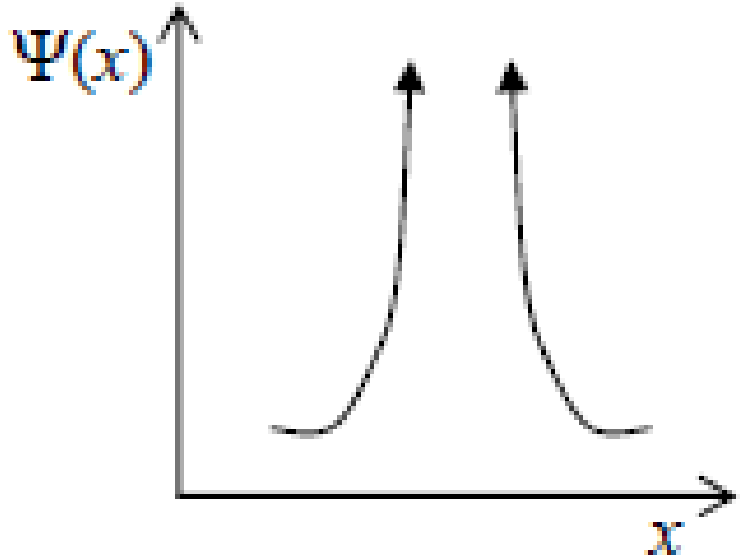

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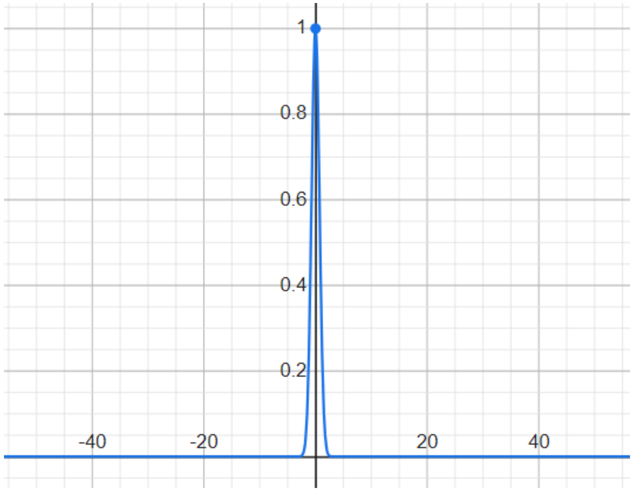
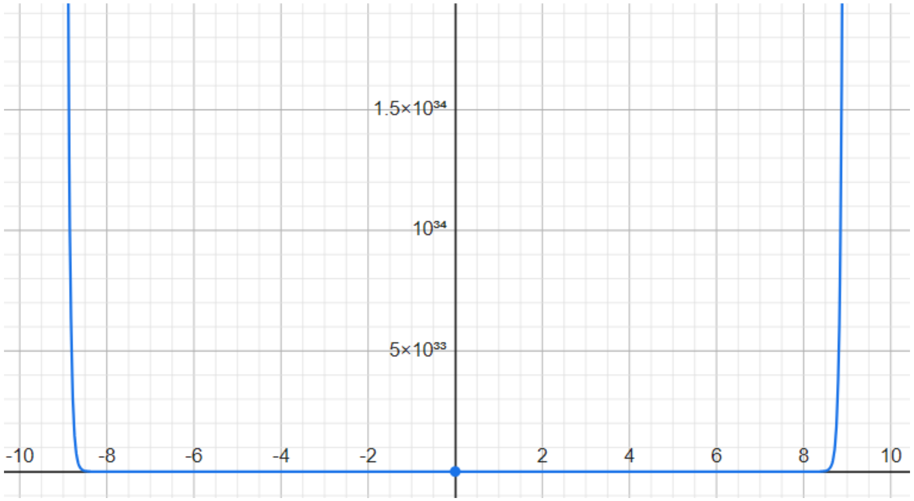


e^{-x^2}

(4)



e^{x^2}

Operator and measurables

$$\hat{A}\,\psi(x) = a\,\psi(x)$$

a is eigenvalue corresponding to $\hat{A}$ operator.
$\psi(x)$ is eigenfunction.

(1) $\psi(x) = A e^{-\frac{x^2}{a^2}}$ $\qquad \hat{A} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ (KE op.)

$$\hat{A}\,\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(A e^{-\frac{x^2}{a^2}}\right)$$

$$= -\frac{\hbar^2}{2m}\frac{d}{dx}\left[-\frac{2A}{a^2}\,x\,e^{-\frac{x^2}{a^2}}\right]$$

$$= \frac{\hbar^2 A}{ma^2}\left[x\left(-\frac{2x}{a^2}e^{-\frac{x^2}{a^2}}\right) + e^{-\frac{x^2}{a^2}}\right]$$

$$\hat{A}\,\psi(x) = \frac{A\hbar^2}{ma^2}\left(1-\frac{2x^2}{a^2}\right)e^{-\frac{x^2}{a^2}}$$

$\longrightarrow$ because of this $\psi(x)$ not an eigenfn.

② $\hat{A} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$ $\psi(x) = Ae^{ikx}$

$$\hat{A}\psi(x) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\left(Ae^{ikx}\right)$$

$$= \frac{-\hbar^2}{2m}(ikA)\frac{d}{dx}\left(e^{ikx}\right)$$

$$= \frac{-\hbar^2}{2m}(ik)^2 A\, e^{ikx}$$

$$= \frac{\hbar^2 k^2}{2m} A e^{ikx}$$

$$\hat{A}\psi(x) = \underbrace{\frac{\hbar^2 k^2}{2m}}_{\text{eigenvalue}} \underbrace{\psi(x)}_{\text{eigenfunction}}$$

Quantity	Operator	Symbol
Position	Multiplication by x	X
Linear momentum (x-component)	$-i\hbar\dfrac{d}{dx}$	P_x
Kinetic energy	$-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$	K
Potential energy	Multiplication by $V(x)$	V
Total mechanical energy	$-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}+V(x)$	H

$\psi^* =$ Conjugate of ψ

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x^2 \psi(x)\, dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, f(x)\, \psi(x)\, dx$$

Operator: Properties

(1) Linear Operator

a) $A[f(x)+g(x)] = Af(x) + Ag(x)$

b) $A[cf(x)] = c[Af(x)]$

e.g. 1) $A = x$ 2) $A =$ squaring

$x[f(x)+g(x)] = xf(x) + xg(x)$

$x[cf(x)] = c[xf(x)]$ ✓

2) $A[f(x)+g(x)] = [f(x)+g(x)]^2$ ✓ —— (i)

$A[f(x)] + A[g(x)] = [f(x)]^2 + [g(x)]^2$ —— (ii)

$(i) \neq (ii)$

2) $A =$ squaring (not a linear operator)

Ques. A particle at $t=0$ is represented by wave fn.

$$\psi(x,0) = \begin{cases} A\dfrac{x}{a}, & 0 \le x \le a, \\ A\dfrac{(b-x)}{(b-a)}, & a \le x \le b, \\ 0, & \text{otherwise} \end{cases}$$

1) Normalise ψ (find A in terms of a and b)

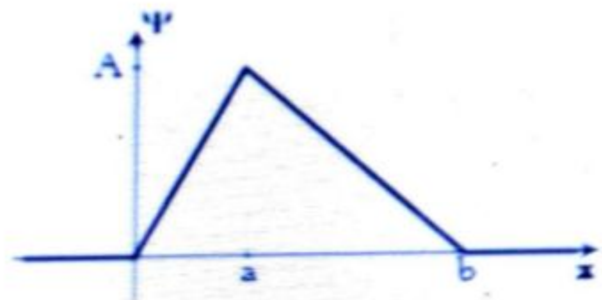
2) Sketch $\psi(x,0)$ as a function of x.

(a)

$$1 = \frac{|A|^2}{a^2}\int_0^a x^2 dx + \frac{|A|^2}{(b-a)^2}\int_a^b (b-x)^2 dx = |A|^2\left\{\frac{1}{a^2}\left(\frac{x^3}{3}\right)\Big|_0^a + \frac{1}{(b-a)^2}\left(-\frac{(b-x)^3}{3}\right)\Big|_a^b\right\}$$

$$= |A|^2\left[\frac{a}{3} + \frac{b-a}{3}\right] = |A|^2\frac{b}{3} \Rightarrow \boxed{A = \sqrt{\frac{3}{b}}.}$$

(b)



Quantum Mechanics: What have we learnt so far??

1. Schrodinger's equation
2. Wave function
3. Acceptable wave function
4. Operators and measurables

Always be happy and grateful