More of Schrodinger, Heisenberg, and Born

Note Title 12-01-2011

Quiz I: January 25, 2011, Tuesday, 1715 hrs

$\underline{\Psi}(\vec{r}, t)$

$\psi(\vec{r})$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi}$$

Operator

eigen value

eigen function

$$\hat{O}_p f = g$$

Eigen value equation

$$\boxed{\hat{O}_p f = \text{constant} \times f}$$

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Kinetic energy operator (in 1-D)

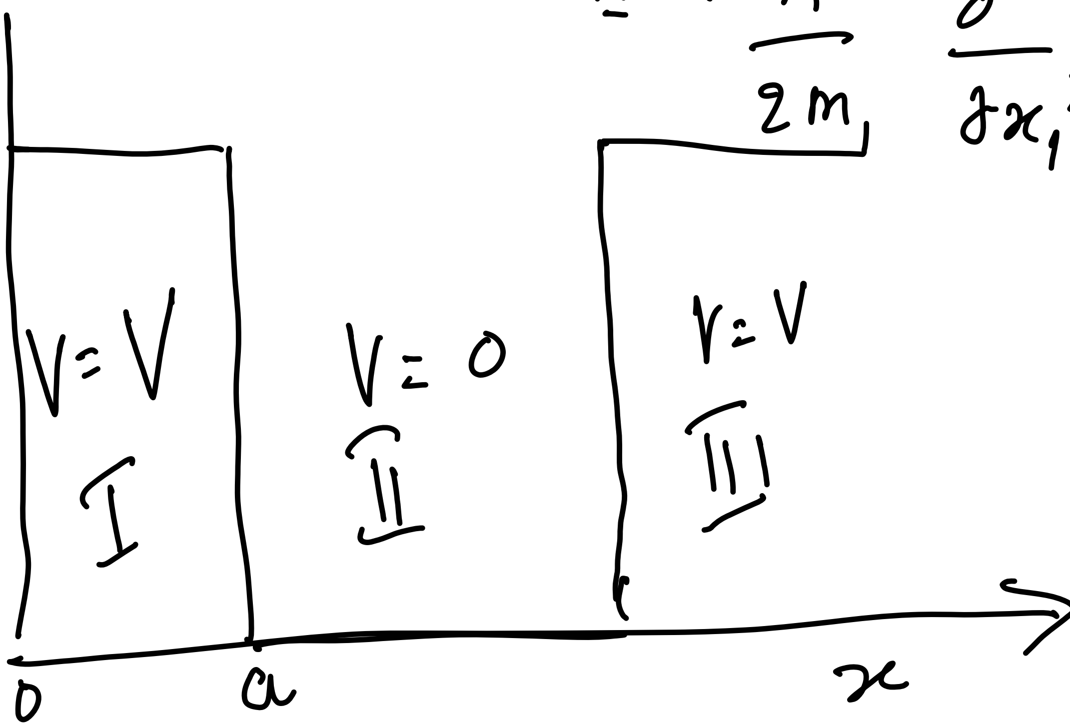
In 3-D $\quad \hat{T} = -\frac{\hbar^2}{2m}\nabla^2$

$$\Big(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\hat{T}} + \underbrace{\hat{V}}_{\hat{V}}\Big)\psi = E\psi$$

n - particles

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \cdots$$



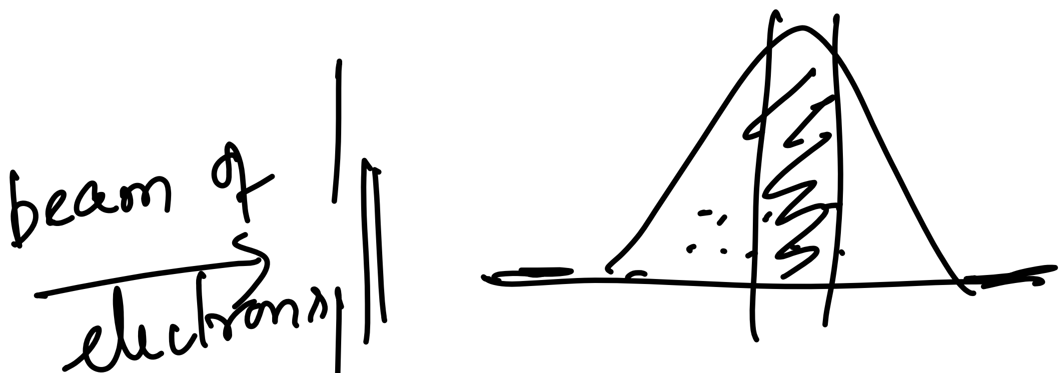
Region I : $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\psi = E\psi$

Region II : $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi = E\psi$

Region III = Region I

ψ → analogy with waves

Born



E

E^2

$|\psi|^2 dx$ — Prob of finding the particle at x & $x+dx$ at time t

Max Born

ψ should be square integrable

ψ and $\frac{d\psi}{dx}$ should be finite, single valued & continuous.

ψ = complex

$$\int |\psi|^2 \, dx = 1$$

Normalization over all space

If ψ is a solution to the SE :

then constant x ψ

$|\psi|^2$

$\downarrow$

$\psi^* \psi$

$\downarrow$

$c^* \psi^* c \psi$

$$\int c^* \psi^* \times c \psi \underbrace{d\tau}_{\text{volume element}} = 1$$

over all space

$e^{i\lambda} c$

$$\underline{\underline{|c|^2}} \int \psi^* \psi \, d\tau = 1 \Big] \text{Normalization}$$

S. E is a linear equation

$\hookrightarrow$ "superposition"

$\psi \rightarrow$ Probabilistic interpretation

$\psi \rightarrow$ Normalized

S.E $\rightarrow$ linear

$$\boxed{\psi \ \& \ \frac{d\psi}{dx} \rightarrow \text{finite, single-valued, \& continuous}}$$

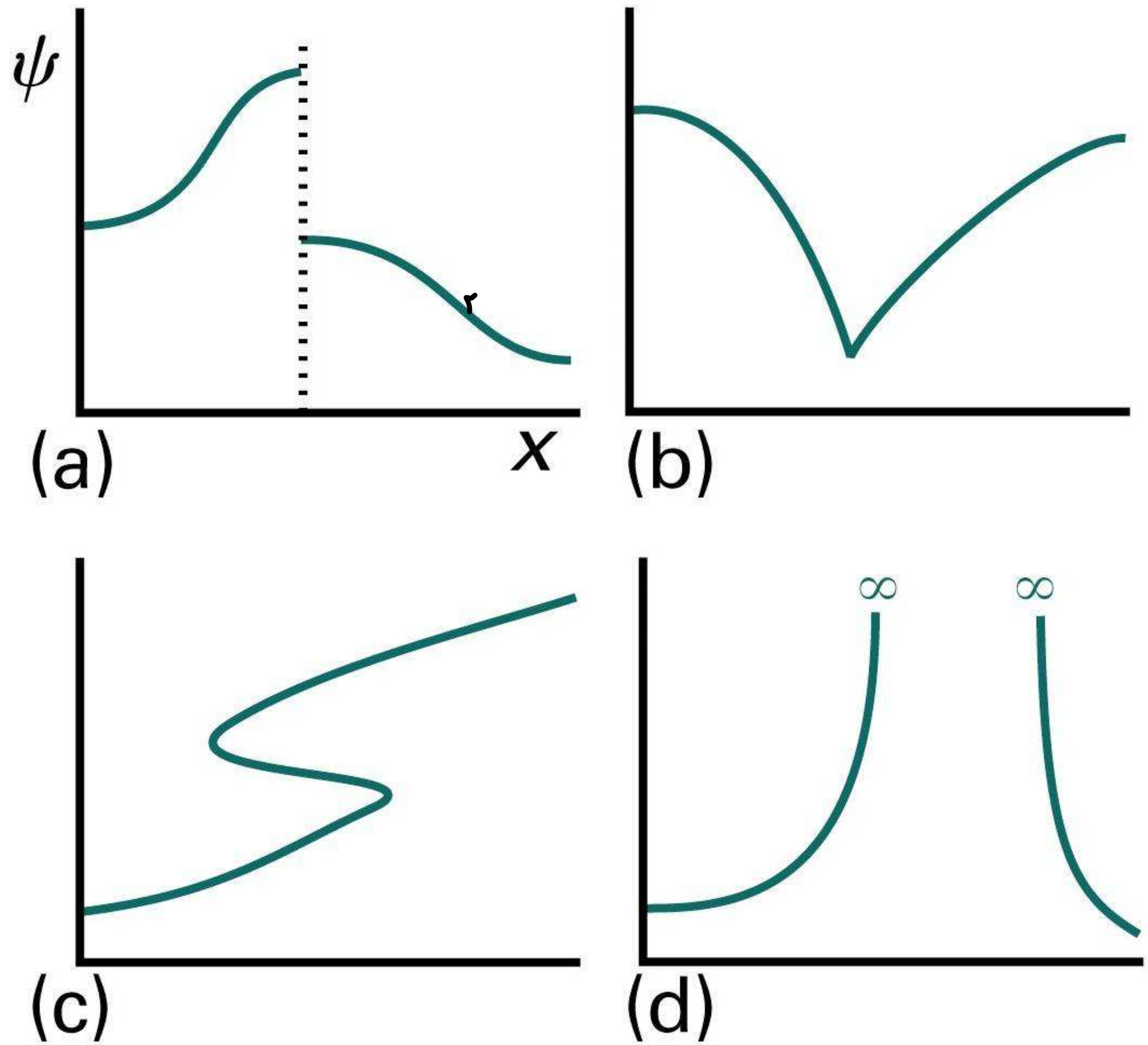
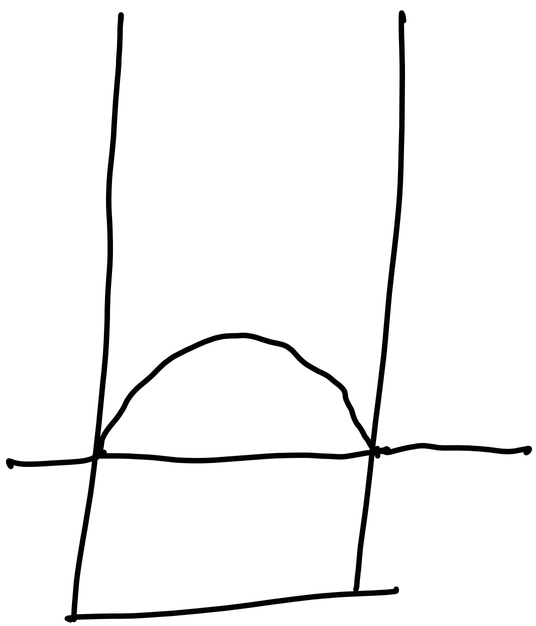


Figure 8-24
Atkins Physical Chemistry, Eighth Edition

Unacceptable as wavefunctions

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi = E\psi$$



$$\frac{d^2\psi}{dx^2} = \frac{2m(V-E)}{\hbar^2}\psi$$

First derivative discontinuous when $V = \infty$

Postulates of Q.M

1) $\Psi(\vec{r}, t) \rightarrow$ Probabilistic interpretation

$$|\Psi|^2 d\tau$$

2) Operator $\longleftrightarrow$ Classical observable

3) Measurement

$$\hat{T}\,\Psi = t_k\,\Psi$$

$\hookrightarrow$ eigen values

4) Expectation value

$$\langle \hat{O} \rangle = \frac{\int \Psi^* \hat{O}\, \Psi\, d\tau}{\int \Psi^* \Psi\, d\tau}$$

E_{1s}, $E_{2s, 2p}$, $E_{3s, 3p, 3d}$, ...

(5)

$$i\hbar \frac{\partial \psi}{\partial t} = \underbrace{\hat{H}}_{\hat{T} + \hat{V}} \psi$$