

Modern Physics (Phys. IV): 2704

Professor Jasper Halekas
Van Allen 70
MWF 12:30-1:20 Lecture

Announcements


- Midterm II in class Wednesday
 - Covers Ch. 5-7 (minus exclusions listed on Friday)
 - Same policies as Midterm I
 - Practice Midterm II solutions now posted

Schrödinger Equation

Time-Dependent

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

U(x) constant
in time



Time-Independent

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

Valid Wave Functions

- $\Psi(x,t) = \psi(x)e^{-i\omega t}$ with $\omega = E/\hbar$ (Time-independent $U(x)$)

$\Psi^*(x,t)\Psi(x,t) =$ probability of finding particle at x at time t
provided the wavefunction is normalized.

$$\int \Psi^* \Psi dr = 1$$

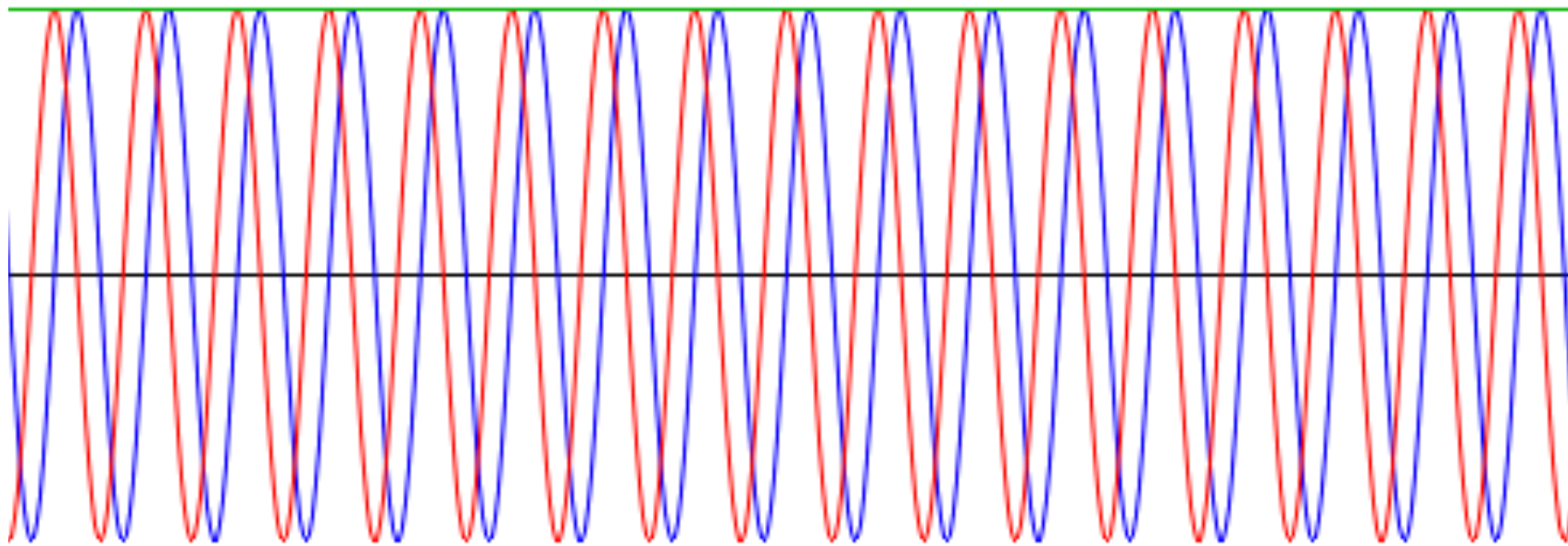
Wave functions must be continuous in value (always)
and in slope (unless the potential energy is infinite).

Traveling Wave: Constant Potential ($E > U_0$)

$$\psi(x) = A_1 \sin(kx) + B_1 \cos(kx)$$

or $\psi(x) = A_2 e^{ikx} + B_2 e^{-ikx}$

$$k = \sqrt{[2m(E-U_0)]/\hbar}$$

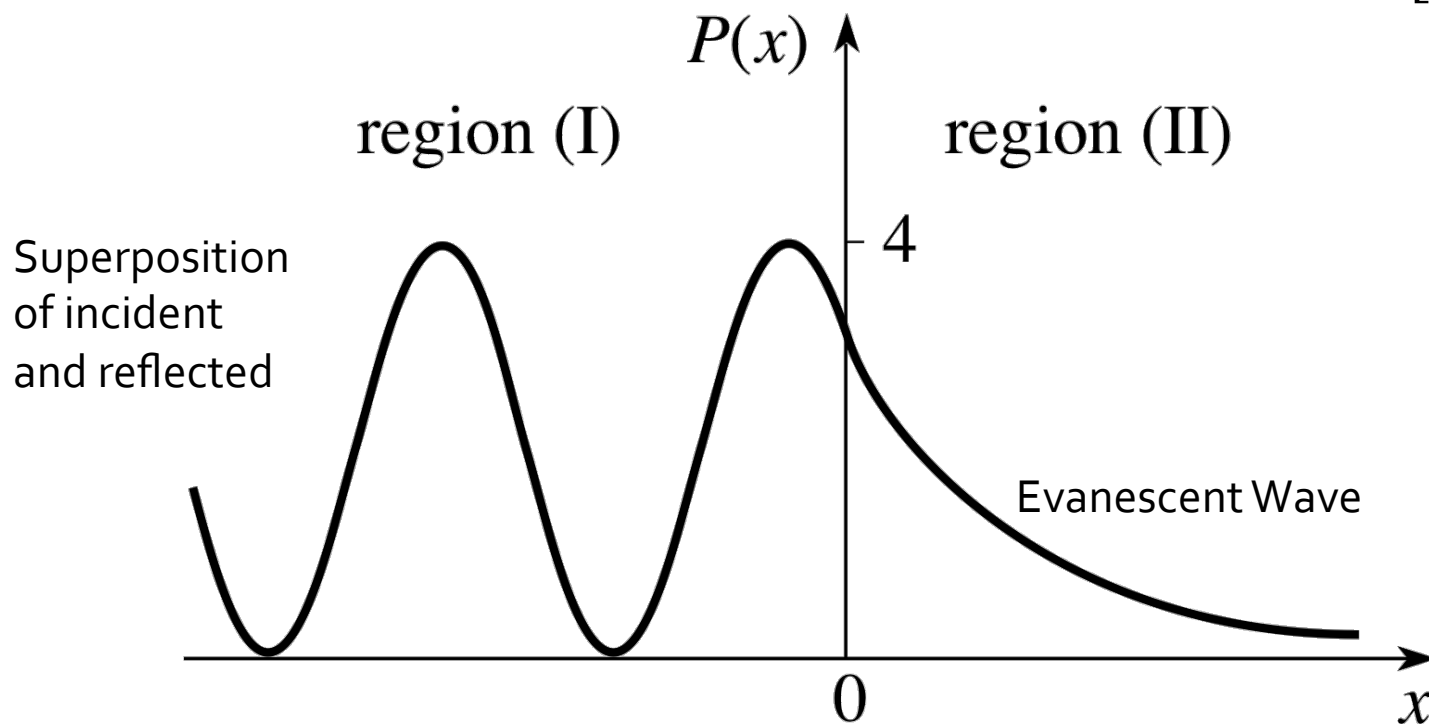


Real, Imaginary, Magnitude

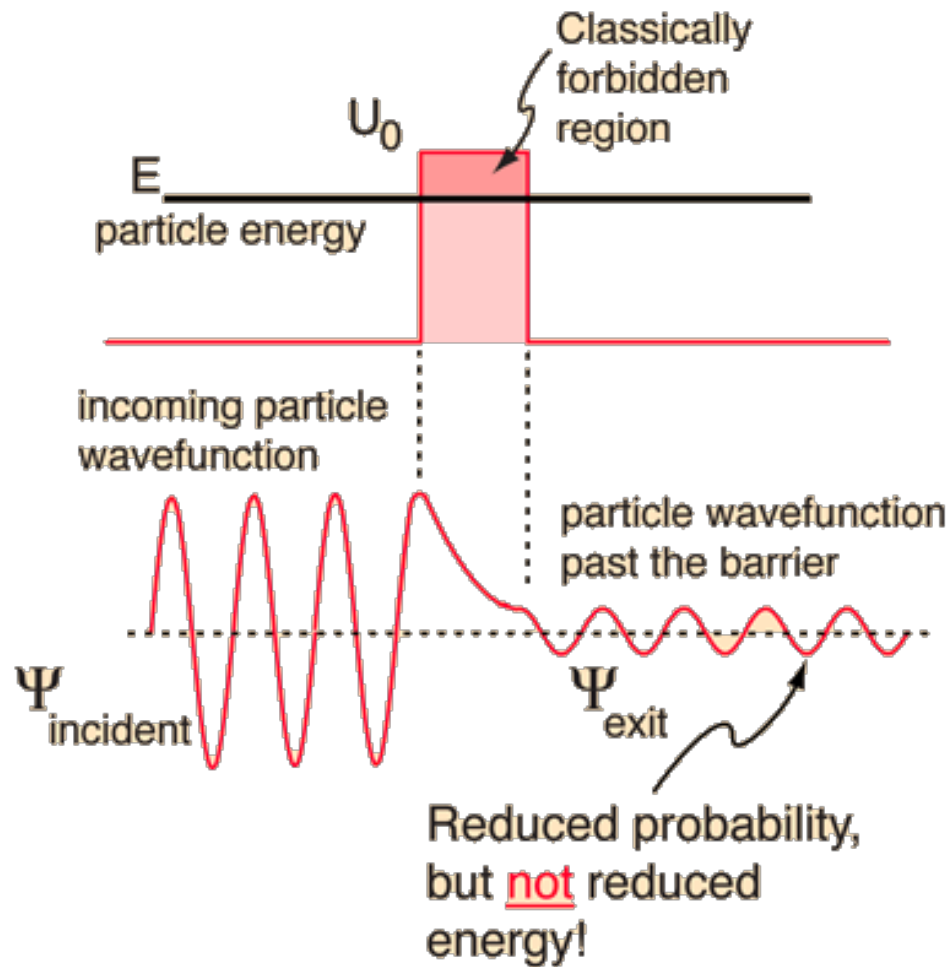
Evanescent Wave: Constant Potential ($E < U_0$)

$$\psi(x) = Ce^{kx} \text{ or } De^{-kx}$$

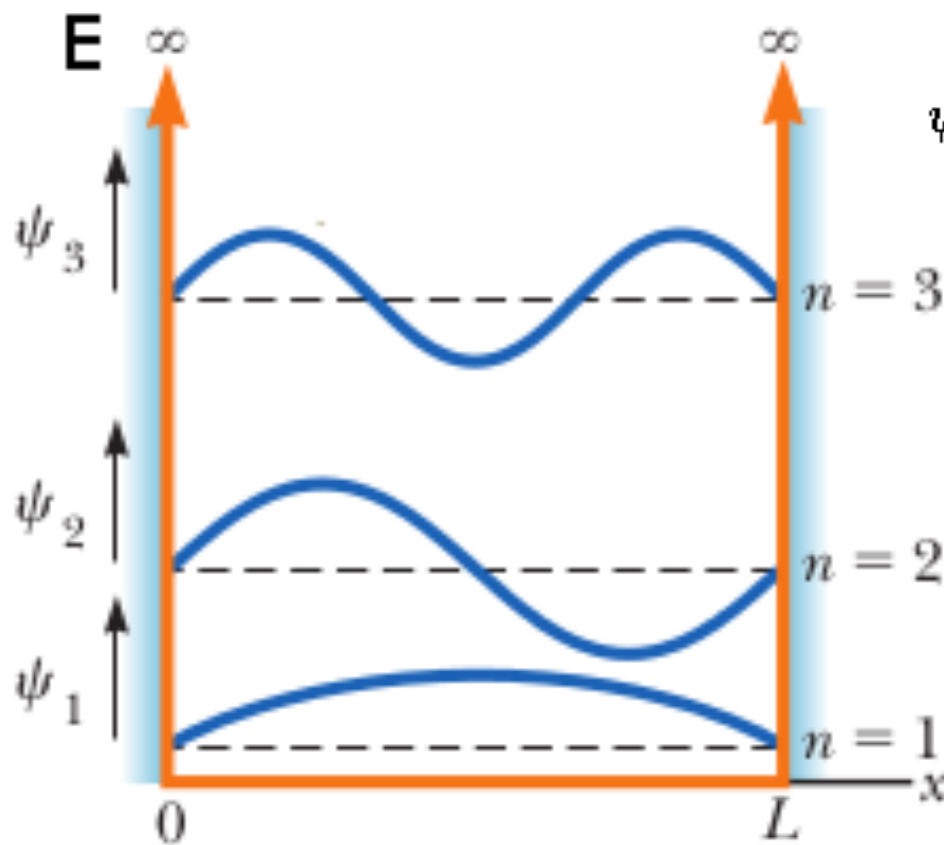
$$k = \sqrt{[2m(U_0 - E)]/\hbar}$$



Tunneling



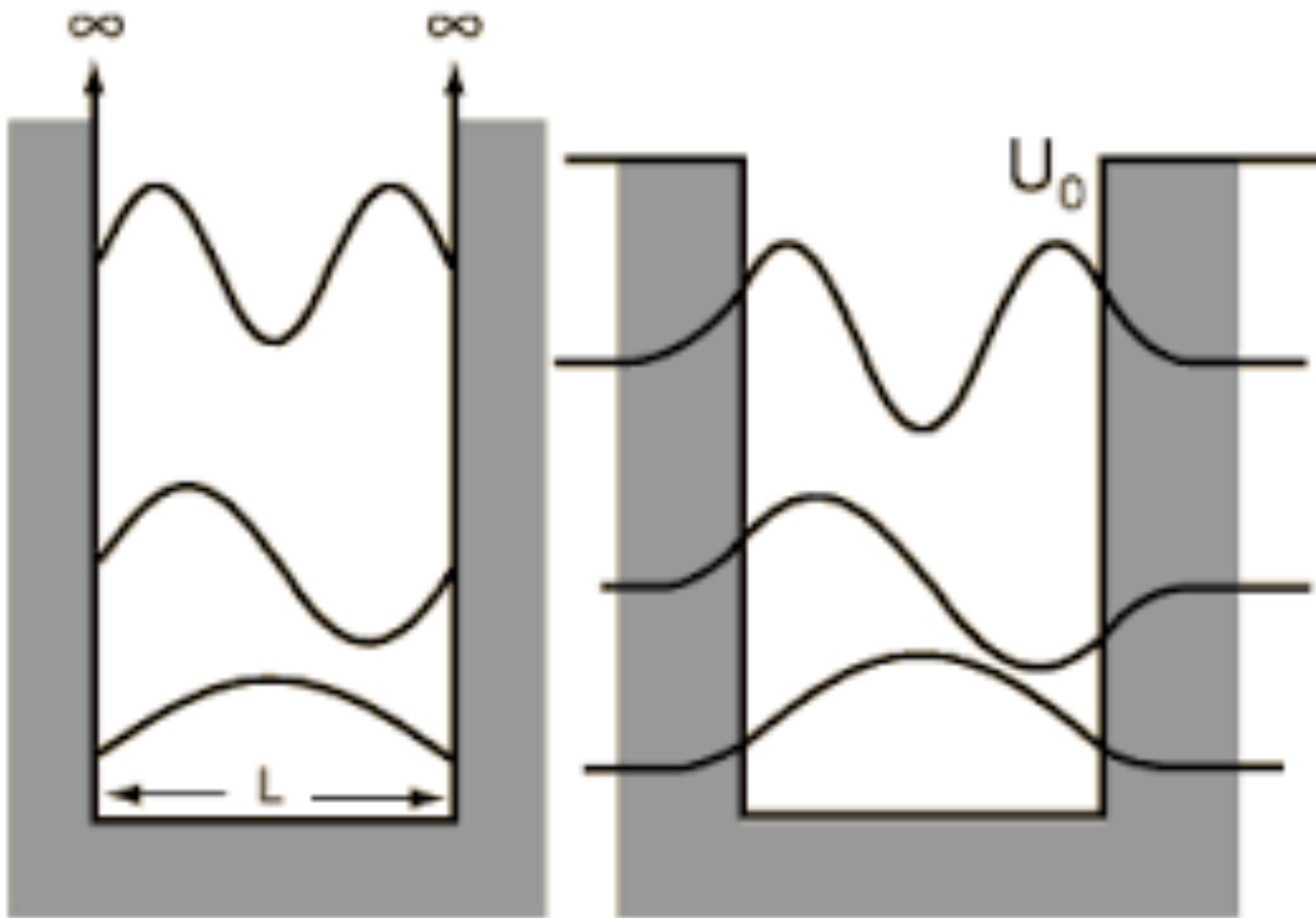
Infinite Square Well



$$\psi(x) = \sqrt{\frac{2}{L}} \sin(k_n x) \quad k_n = \frac{\pi n}{L}$$

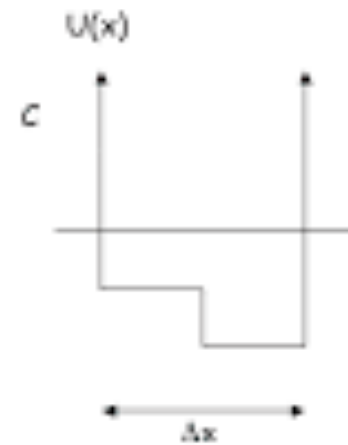
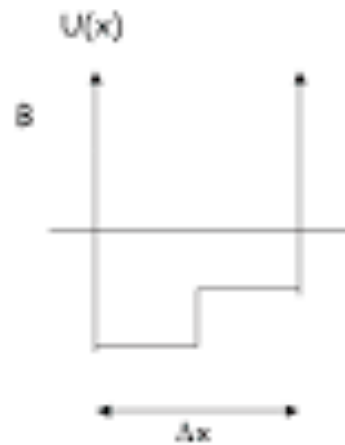
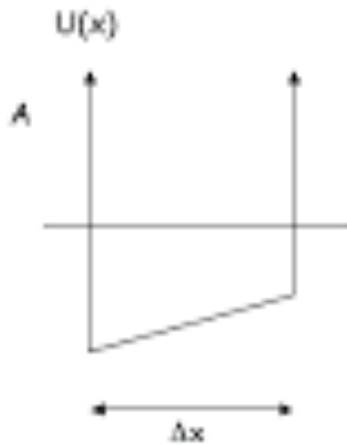
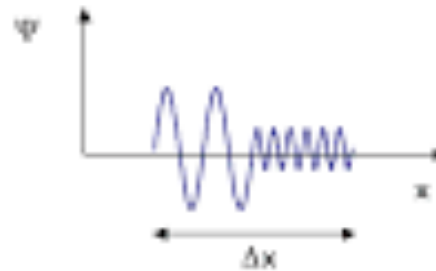
$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

Infinite \rightarrow Finite Square Well



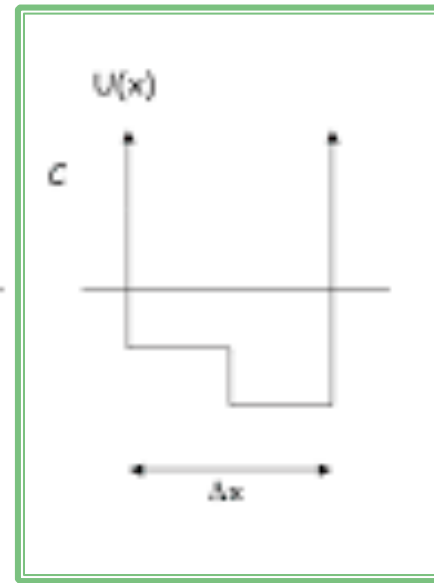
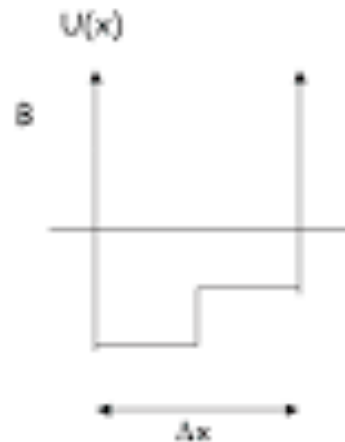
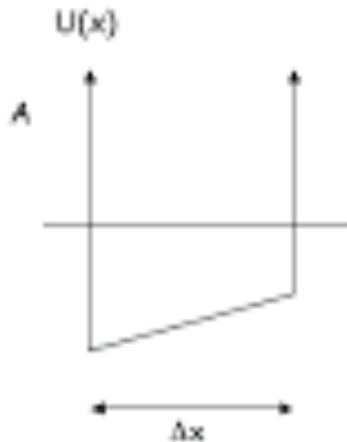
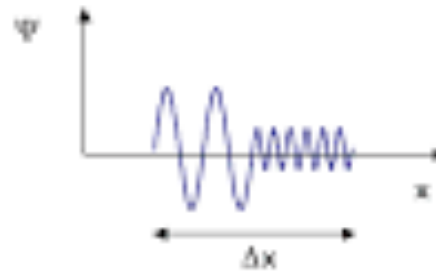
Concept Check

Which potential well would this wave function make sense for?

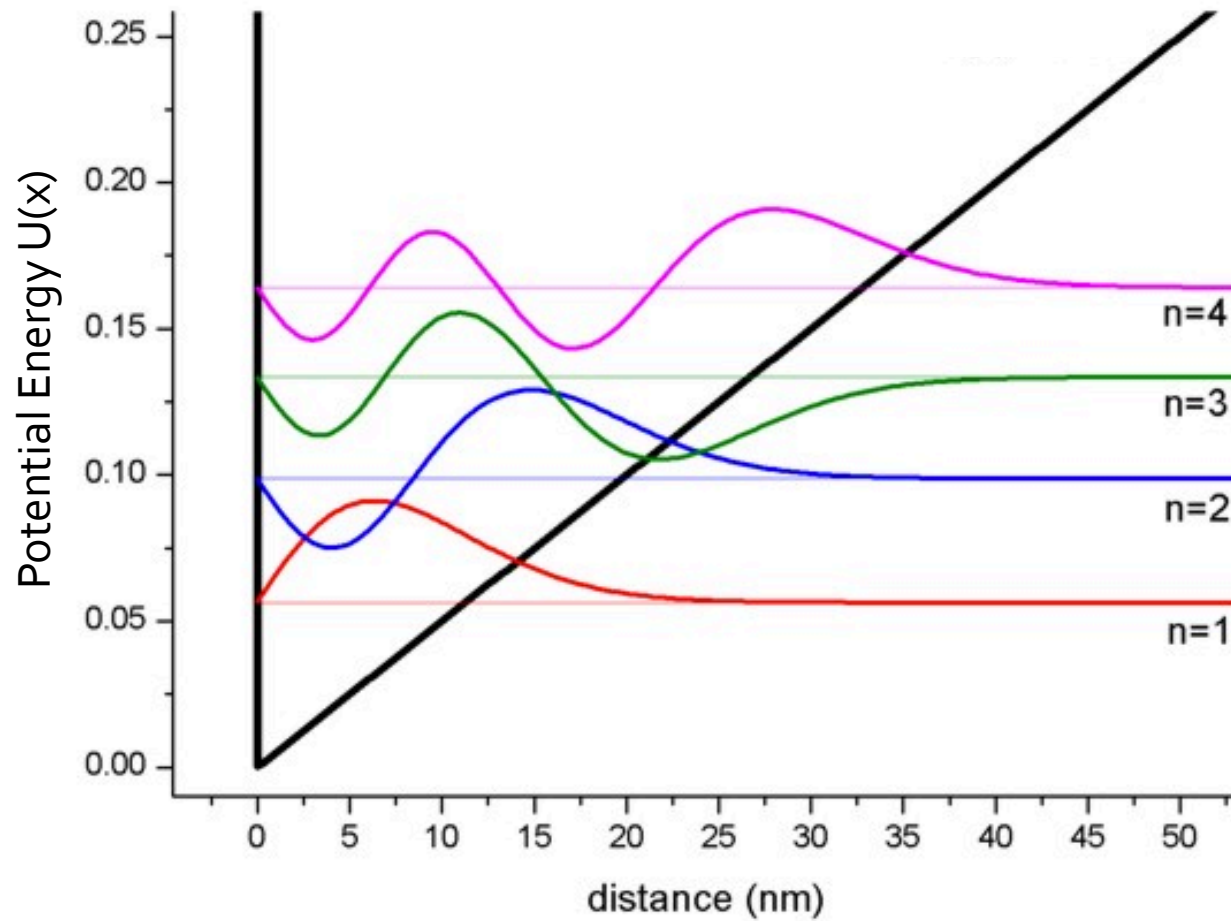


Concept Check

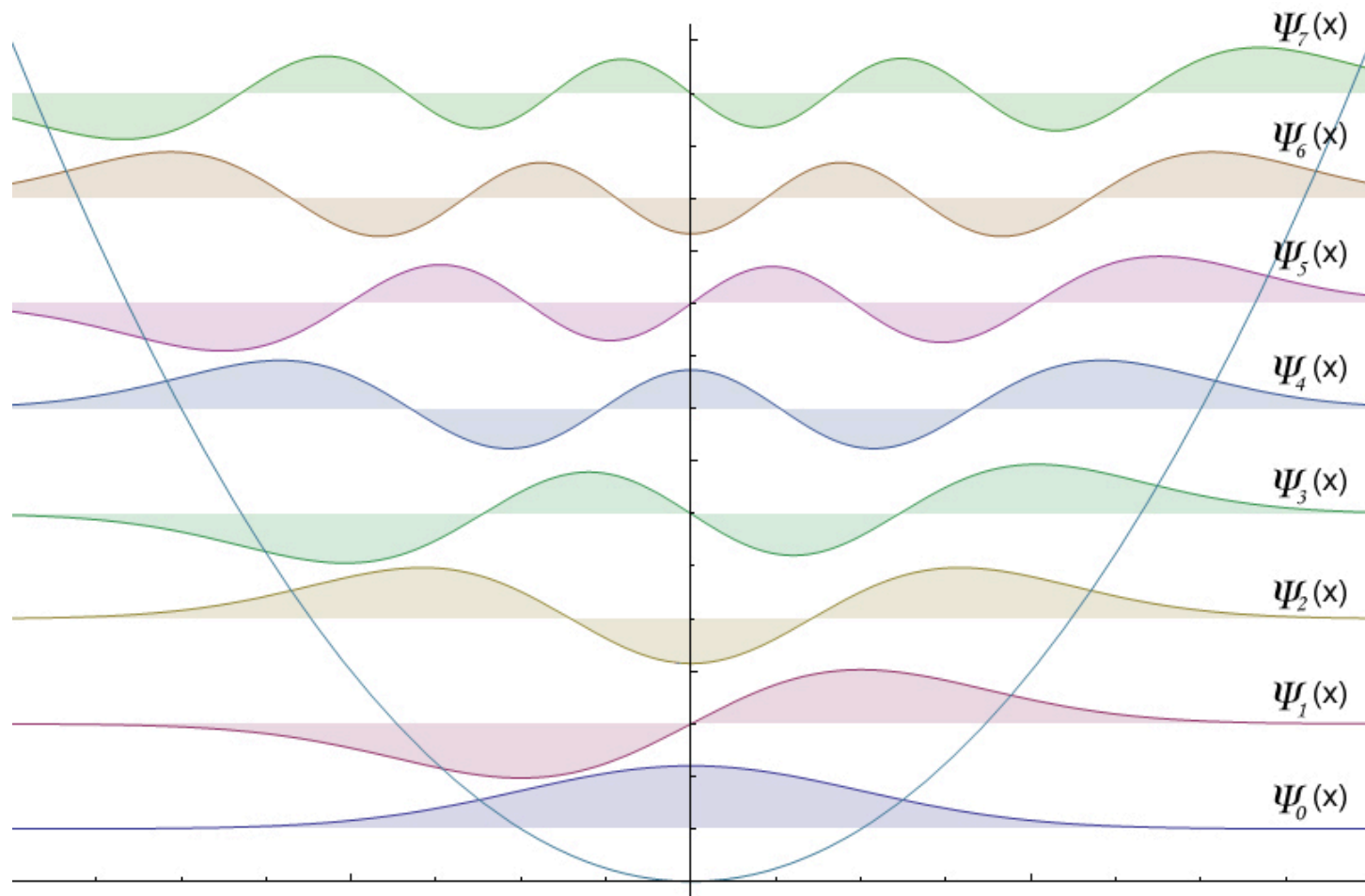
Which potential well would this wave function make sense for?



Asymmetric Well



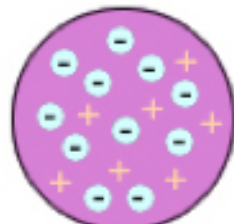
Harmonic Oscillator



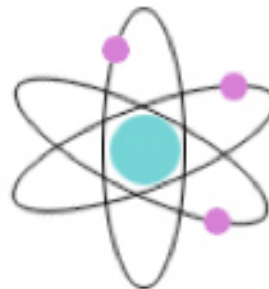
Atomic Models



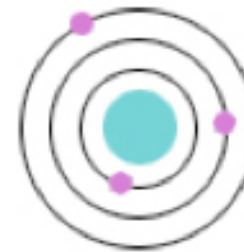
Dalton
"Billiard Ball" Model



Thomson
"Plum Pudding" Model



Rutherford Model

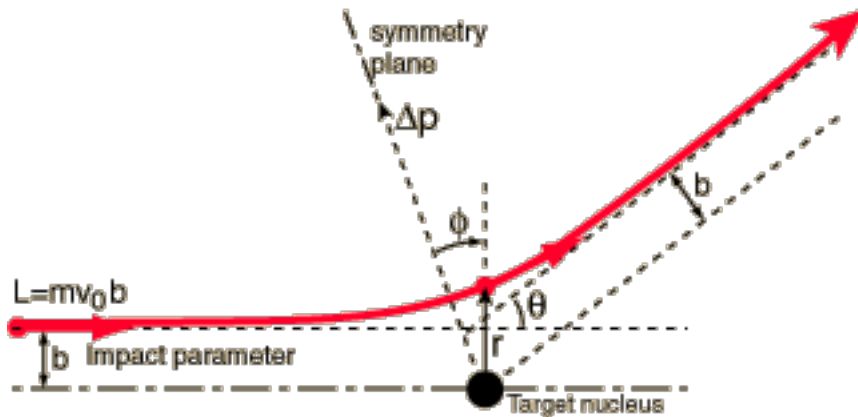


Bohr Model



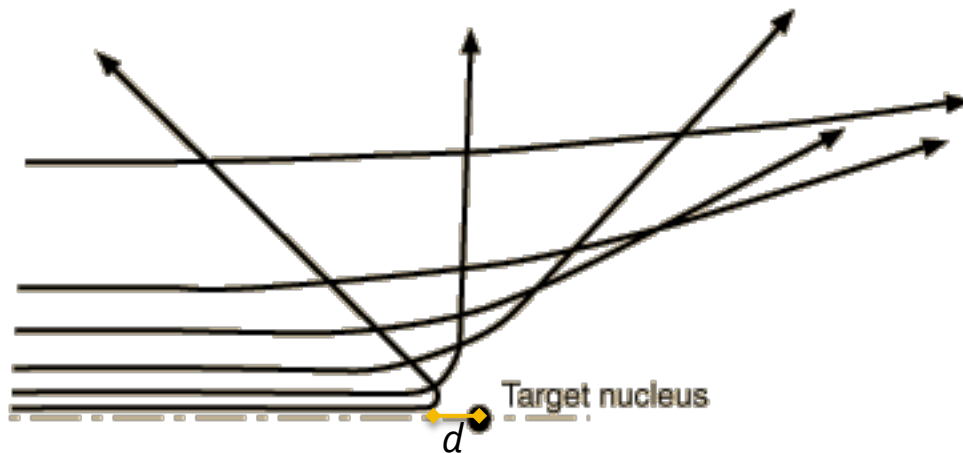
Quantum Mechanical
Model

Rutherford Scattering



Impact Parameter

$$b = \frac{1}{4\pi\epsilon_0} \cdot \frac{Ze^2 \cot \frac{\theta}{2}}{E} \cdot \frac{z}{2}$$

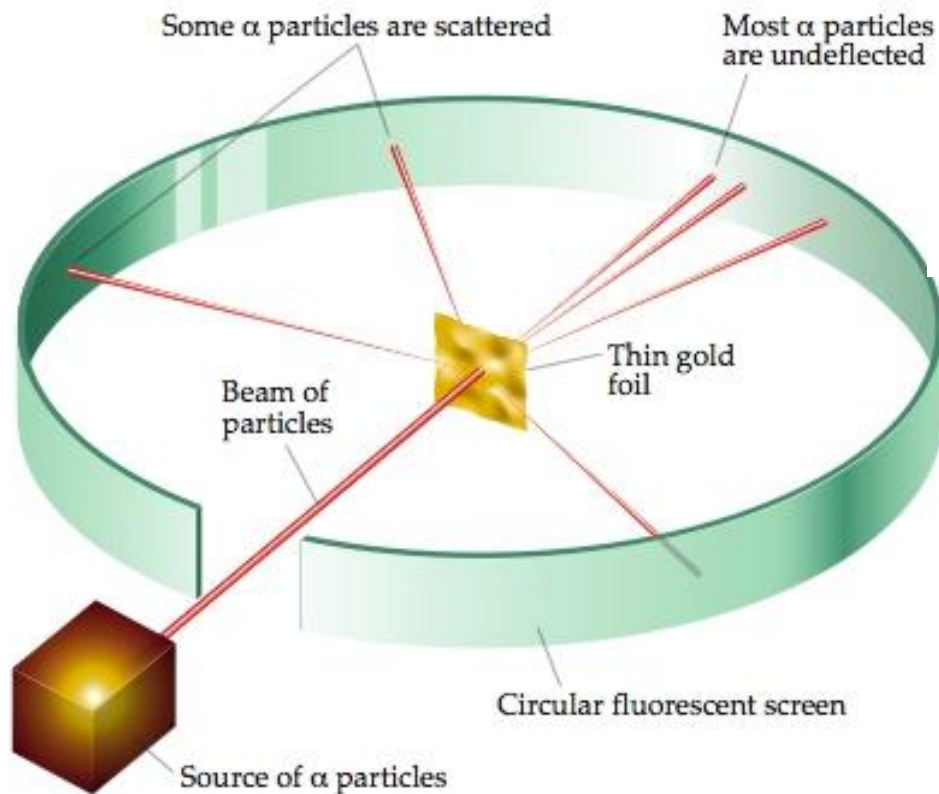


Closest Approach ($b=0$)

$$E = \frac{1}{2}mv^2 = \frac{1}{4\pi\epsilon_0} \frac{z eZe}{d}$$

$$d = \frac{z Ze^2}{4\pi\epsilon_0 K}$$

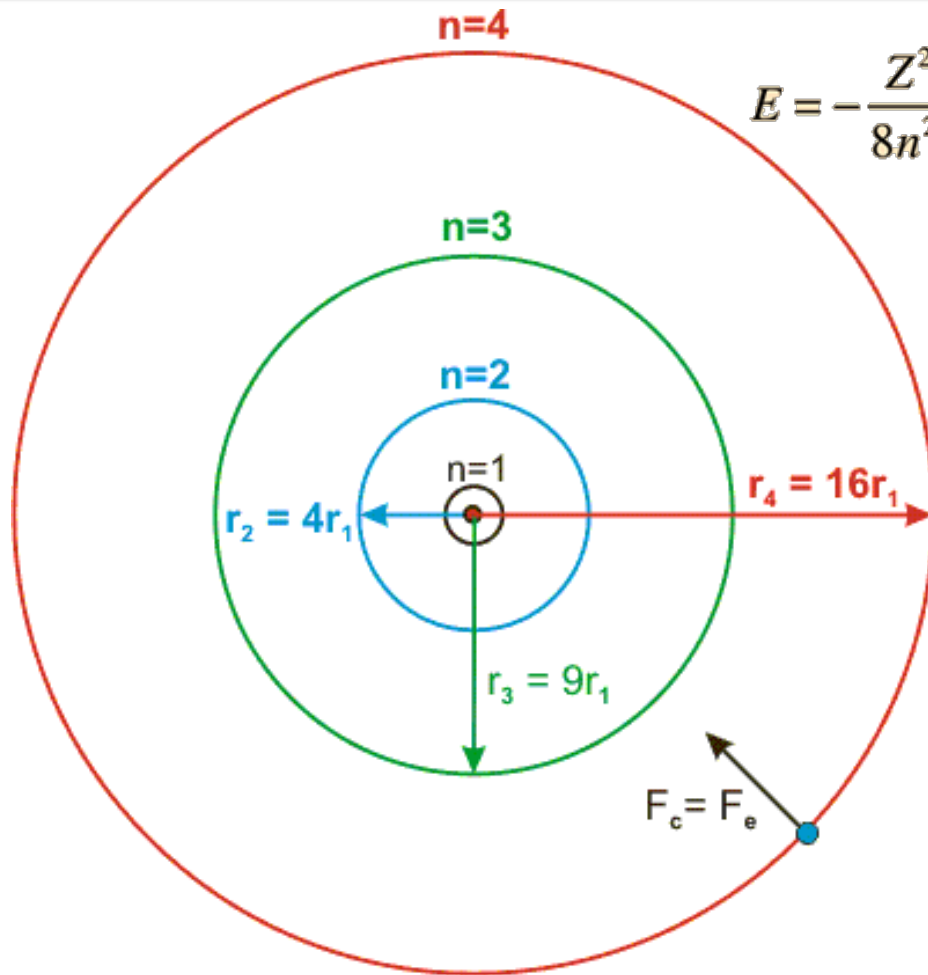
Rutherford Scattering



$$N(\theta) = \frac{nt}{4r^2} \left(\frac{zZ}{2K} \right)^2 \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{\sin^4(\frac{1}{2}\theta)}$$

N = scattered flux
 n = target density
 t = thickness of target
 r = detector distance
 K = projectile energy
 θ = scattering angle

Bohr Model for Hydrogenic Atoms



$$E = -\frac{Z^2 m e^4}{8 n^2 h^2 \epsilon_0^2} = \frac{-13.6 Z^2}{n^2} eV$$

$$r = \frac{n^2 h^2 \epsilon_0}{Z \pi m e^2} = \frac{n^2 a_0}{Z}$$

$$a_0 = 0.0529 \text{ nm} = \text{Bohr radius}$$

Bohr model works for atoms (or ions) with only one electron

Assumes circular orbits, with angular momentum $L = n\hbar$

Not consistent with wavelike nature of electrons

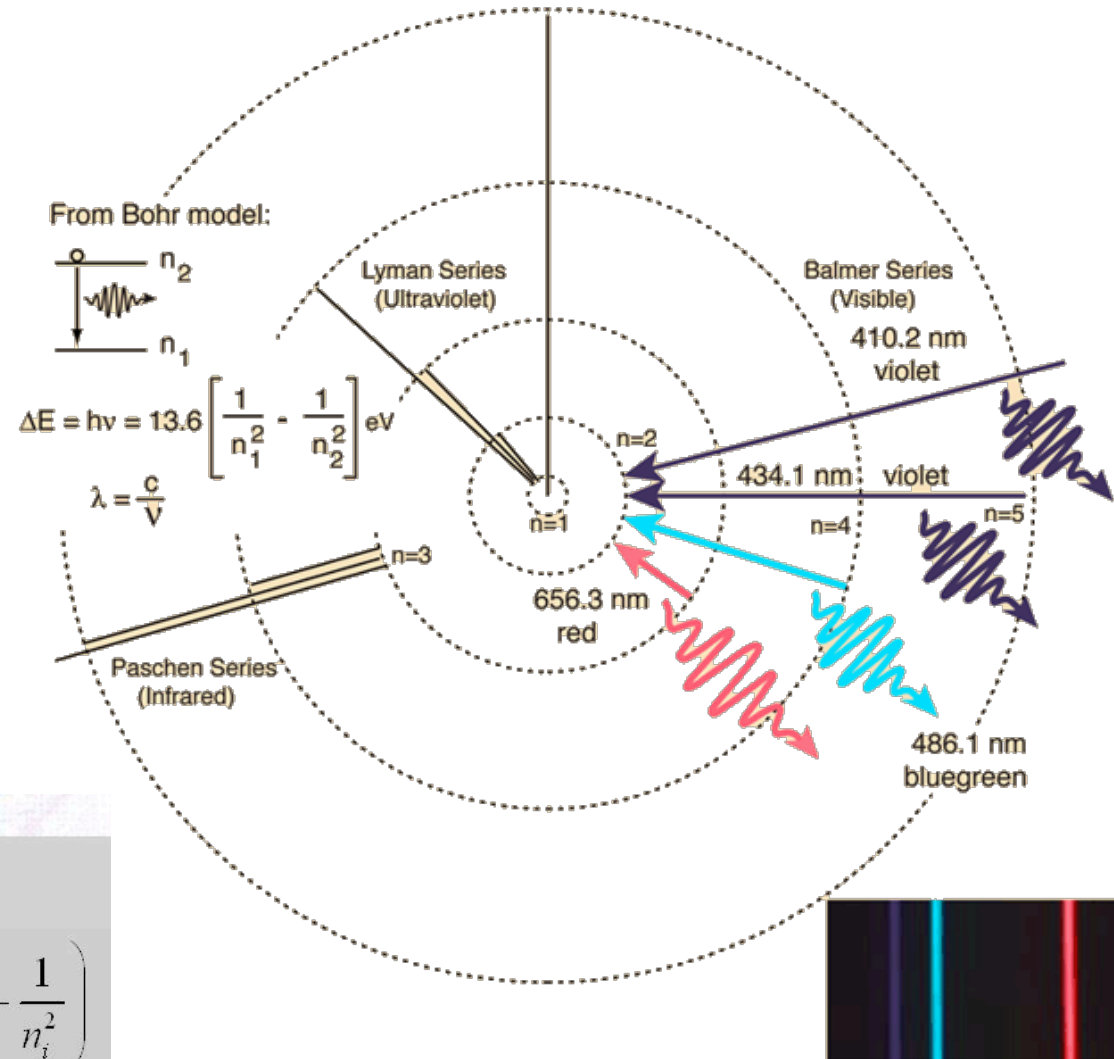
Violates uncertainty principle

Emission/Absorption Spectrum

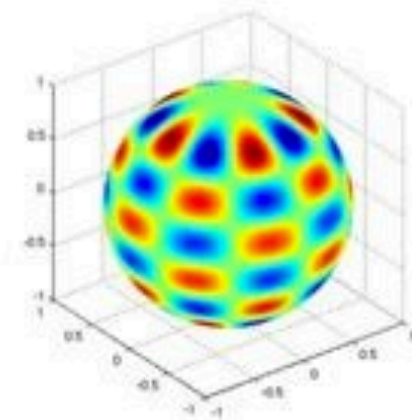
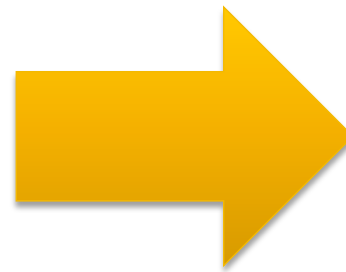
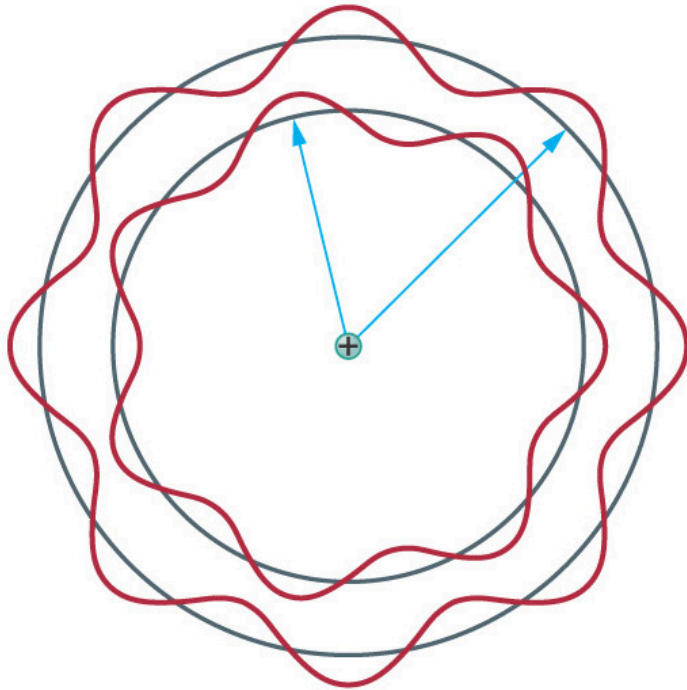
$$h\nu = \frac{Z^2 m_e e^4}{8h^2 \epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$$\frac{1}{\lambda} = \frac{\nu}{c} = \frac{E_i - E_f}{ch} = \frac{E_0}{ch} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$= \frac{m_e e^4}{4c\pi\hbar^3 (4\pi\epsilon_0)^2} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \equiv R_\infty \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$



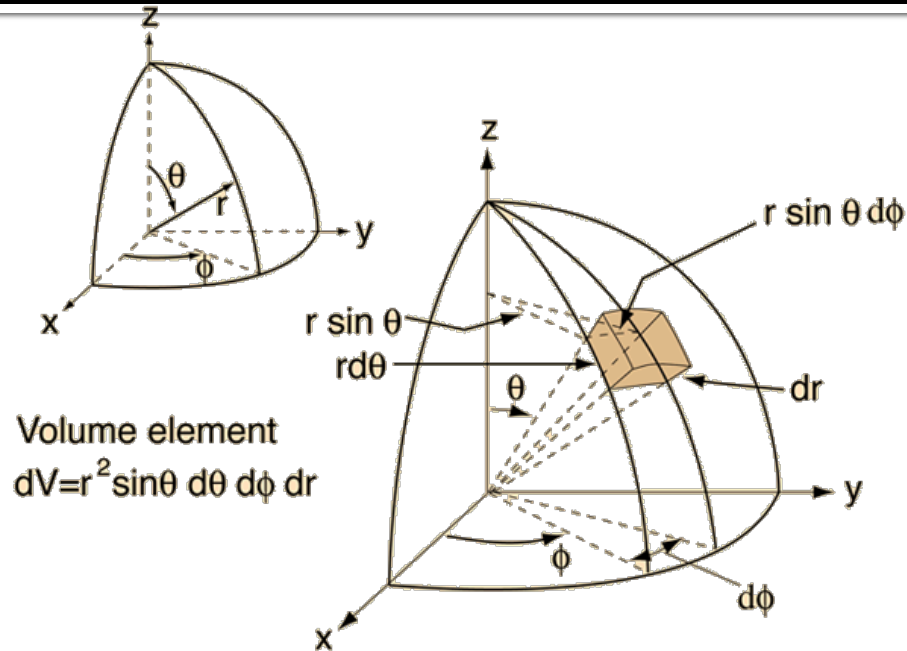
From 1-d to 3-d Standing Waves!



$$\ell = 10$$

$$m = 5$$

Spherical Schrödinger Equation



r (radial): 0 to ∞
 θ (polar): 0 to π
 ϕ (azimuthal): 0 to 2π

$$\begin{aligned}
 & \frac{-\hbar^2}{2\mu} \frac{1}{r^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right] \\
 & + U(r) \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi)
 \end{aligned}$$

Hydrogen Atom: Separation of Variables Solution

$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

$$\Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

n ℓ m_ℓ

principal orbital magnetic
quantum quantum quantum
number number number

$$\Phi(\phi) = A e^{im_\ell \phi} \quad m_\ell = -\ell, -\ell + 1, \dots, +\ell$$

$$\Theta_{\ell m}(\theta) = N_{\ell m} P_n^m(\cos \theta) \quad \ell = 0, 1, 2, 3, \dots, n-1$$

$$R_{n, \ell} = r^\ell L_{n, \ell} e^{-r/na_0} \quad n = 1, 2, 3, \dots$$

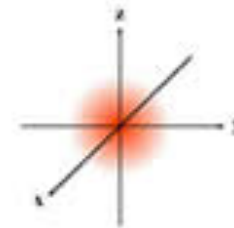
Quantum Numbers and Electron Orbital Properties

$$E_n = \frac{-me^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} = \frac{-13.6eV}{n^2} \quad n = 1, 2, 3, \dots$$

$$L^2 = \ell(\ell + 1)\hbar^2$$

$$L_z = m_\ell \hbar$$

$$S_z = m_s \hbar, \quad m_s = \pm \frac{1}{2}$$



n = principal

distance
from nucleus

Energy

l = angular

shape
of orbital

Orbital
Angular
Momentum

m = magnetic

orientation
in space

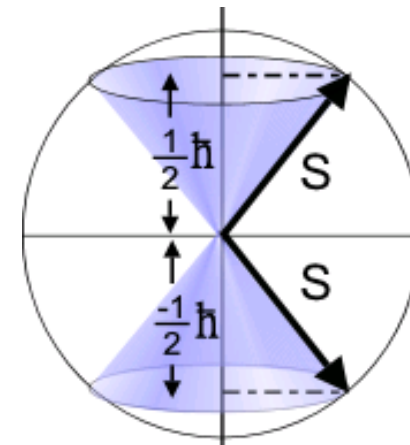
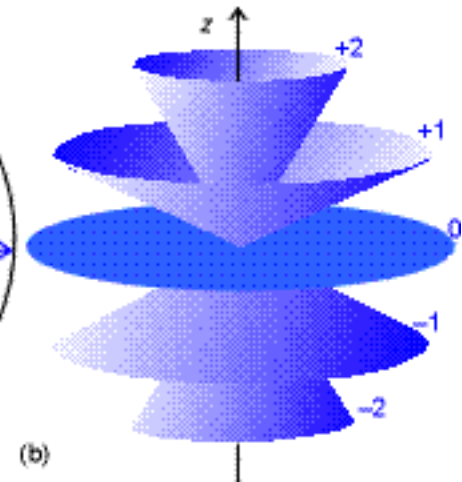
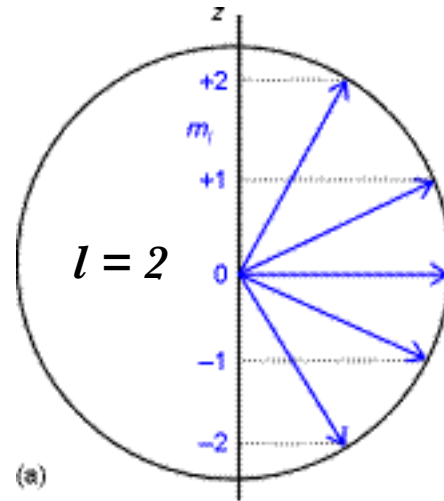
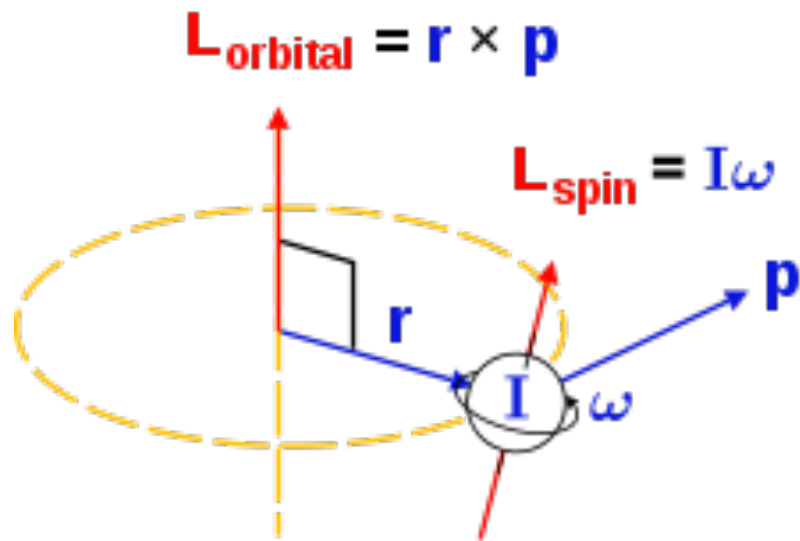
Direction of
Orbital
Angular
Momentum

S = spin

electron
spin

Rotational
Angular
Momentum

Angular Momentum



Concept Check

- Consider an electron in the $l = 2, m_l = 2$ orbital. Where would this electron be most likely to be found?
 - A. Near the z-axis
 - B. Near the x-y plane
 - C. Equally likely to be found anywhere
 - D. Not enough information

Concept Check

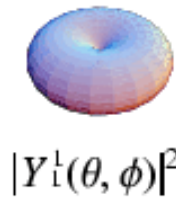
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Angular Probability Distribution

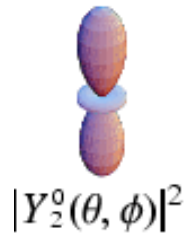
s: l = 0



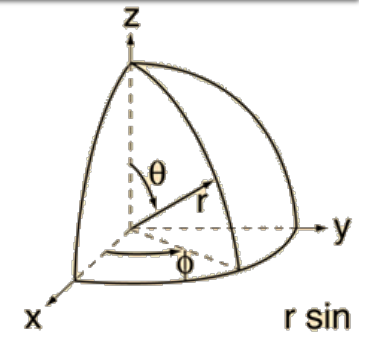
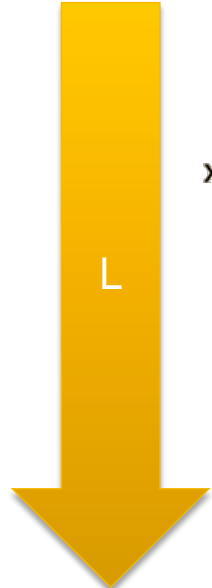
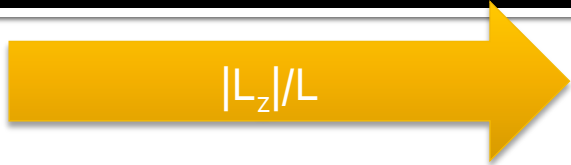
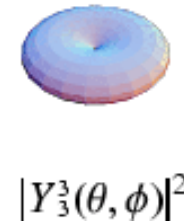
p: l = 1



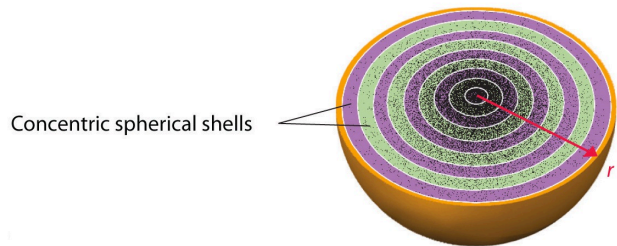
d: l = 2



f: l = 3



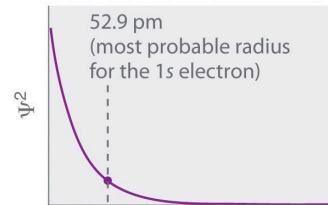
Radial Probability Distribution



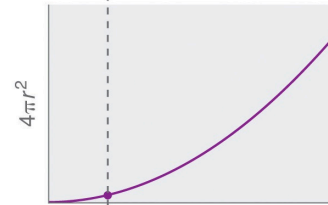
Concentric spherical shells

(a) 1s orbital imagined as an onion

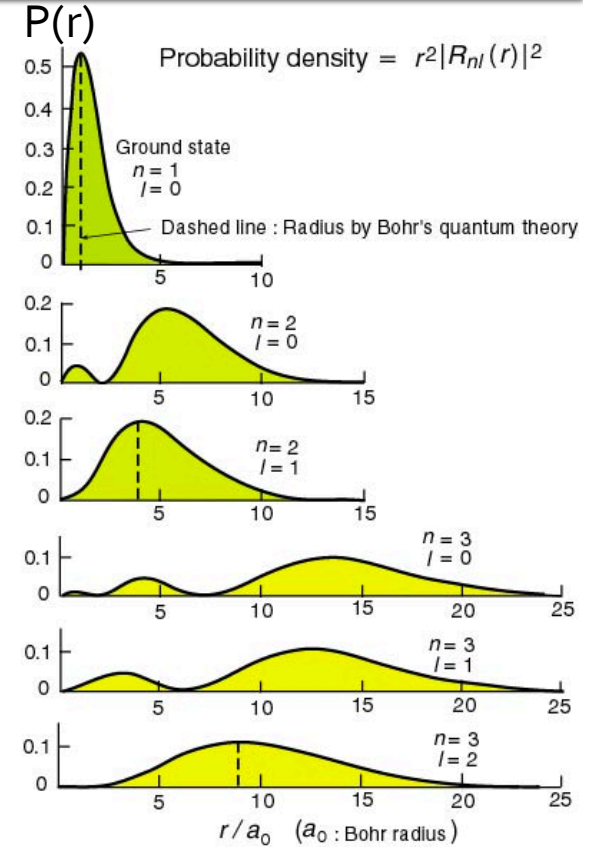
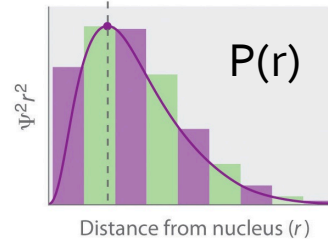
(b) Probability density



(c) Spherical surface area



(d) Radial probability



Maximum probability radius where $d/dr (P(r)) = 0$

Average radius: $\langle r \rangle = \int_0^{\infty} rP(r)dr$