

PHYS 3313 – Section 001

Lecture #17

Monday, Nov. 11, 2013

Dr. Jaehoon Yu

- Alpha Particle Decay
- Use of Schrodinger Equation on Hydrogen Atom
- Solutions for Schrodinger Equation for Hydrogen Atom
- Quantum Numbers
- Principal Quantum Number
- Orbital Angular Momentum Quantum Number
- Magnetic Quantum Number

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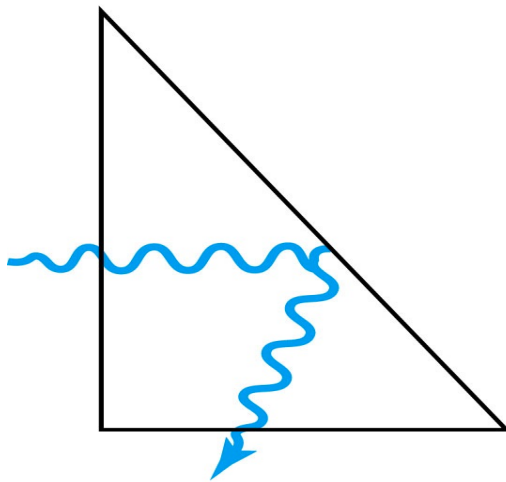
Announcements

- Reminder: homework #6
 - CH6 end of chapter problems: 34, 39, 46, 62 and 65
 - Due on Monday, Nov. 18, in class
- Reading assignments
 - CH7.6 and the entire CH8

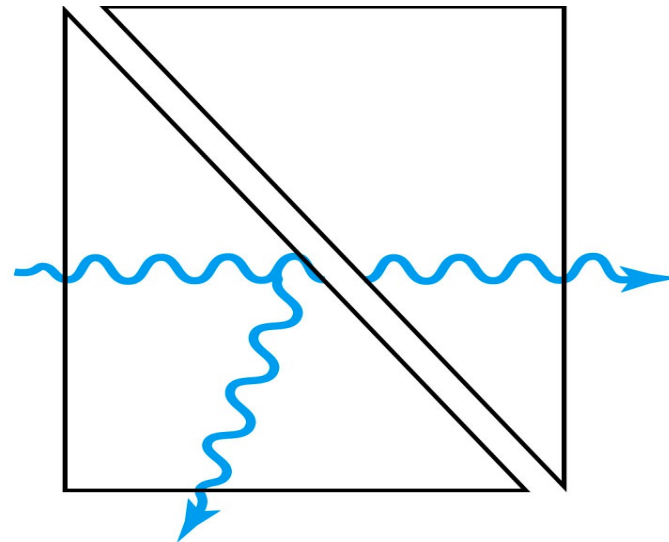


Analogy with Wave Optics

- If light passing through a glass prism reflects from an internal surface with an angle greater than the critical angle, total internal reflection occurs. The electromagnetic field, however, is not exactly zero just outside the prism. Thus, if we bring another prism very close to the first one, experiments show that the electromagnetic wave (light) appears in the second prism.
- The situation is analogous to the tunneling described here. This effect was observed by Newton and can be demonstrated with two prisms and a laser. The intensity of the second light beam decreases exponentially as the distance between the two prisms increases.

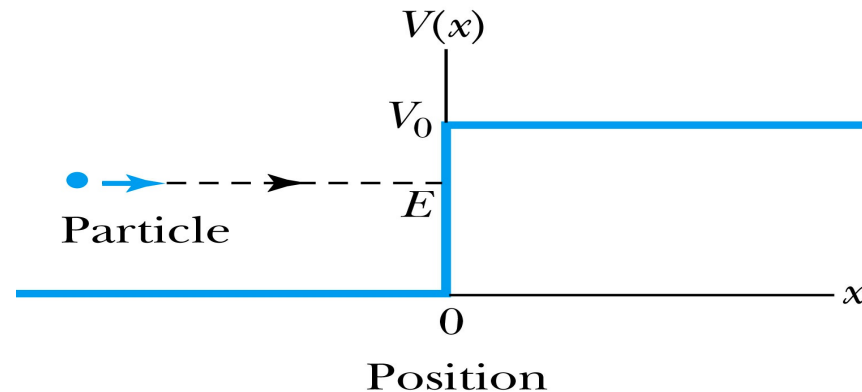


(a)



(b)

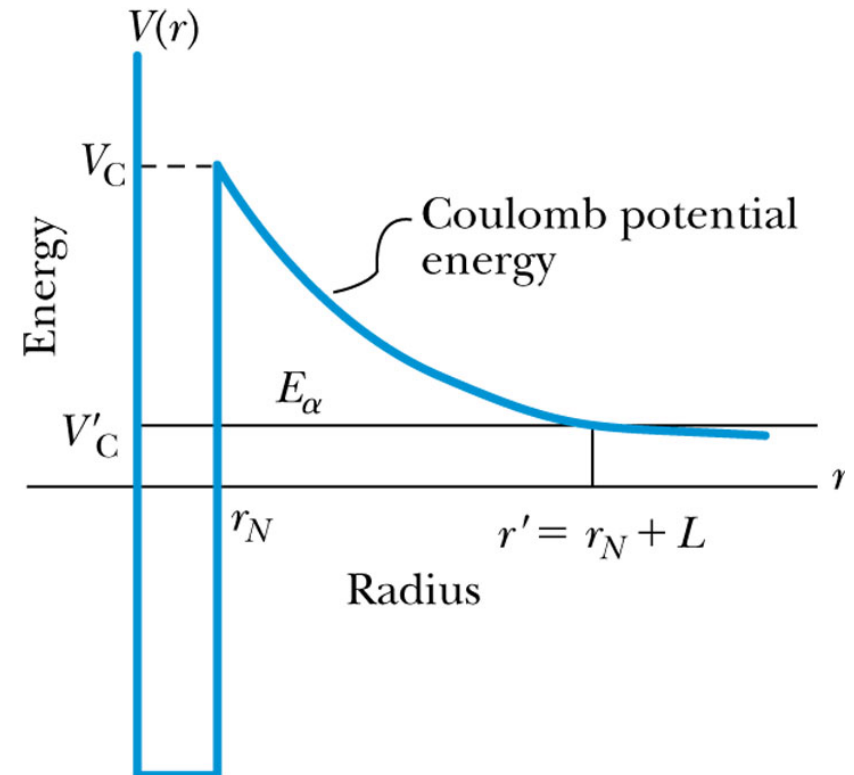
Potential Well



- Consider a particle passing through a potential well region rather than through a potential barrier.
- Classically, the particle would speed up passing the well region, because $K = mv^2 / 2 = E - V_0$. According to quantum mechanics, reflection and transmission may occur, but the wavelength inside the potential well is shorter than outside. When the width of the potential well is precisely equal to half-integral or integral units of the wavelength, the reflected waves may be out of phase or in phase with the original wave, and cancellations or resonances may occur. The reflection/cancellation effects can lead to almost pure transmission or pure reflection for certain wavelengths. For example, at the second boundary ($x = L$) for a wave passing to the right, the wave may reflect and be out of phase with the incident wave. The effect would be a cancellation inside the well.

Alpha-Particle Decay

- Many nuclei heavier than Pb emit alpha particles (nucleus of He)! The phenomenon of tunneling explains the alpha-particle decay of heavy, radioactive nuclei.
- Inside the nucleus, an alpha particle feels the strong, short-range attractive nuclear force as well as the repulsive Coulomb force.
- The nuclear force dominates inside the nuclear radius where the potential is approximately a square well.
- The Coulomb force dominates outside the nuclear radius.
- The potential barrier at the nuclear radius is several times greater than the energy of an alpha particle ($\sim 5\text{MeV}$).
- According to quantum mechanics, however, the alpha particle can “tunnel” through the barrier. Hence this is observed as radioactive decay.



Application of the Schrödinger Equation to the Hydrogen Atom

- The approximation of the potential energy of the electron-proton system is the Coulomb potential:

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

- To solve this problem, we use the three-dimensional time-independent Schrödinger Equation.

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x,y,z)} \left(\frac{\partial^2 \psi(x,y,z)}{\partial x^2} + \frac{\partial^2 \psi(x,y,z)}{\partial y^2} + \frac{\partial^2 \psi(x,y,z)}{\partial z^2} \right) = E - V(r)$$

- For Hydrogen-like atoms with one electron (He^+ or Li^{++})
 - Replace e^2 with Ze^2 (Z is the atomic number)
- Use appropriate reduced mass μ $\left(\mu = \frac{m_1 m_2}{m_1 + m_2} \right)$

Application of the Schrödinger Equation

- The potential (central force) $V(r)$ depends on the distance r between the proton and electron.

$$x = r \sin \theta \cos \phi$$

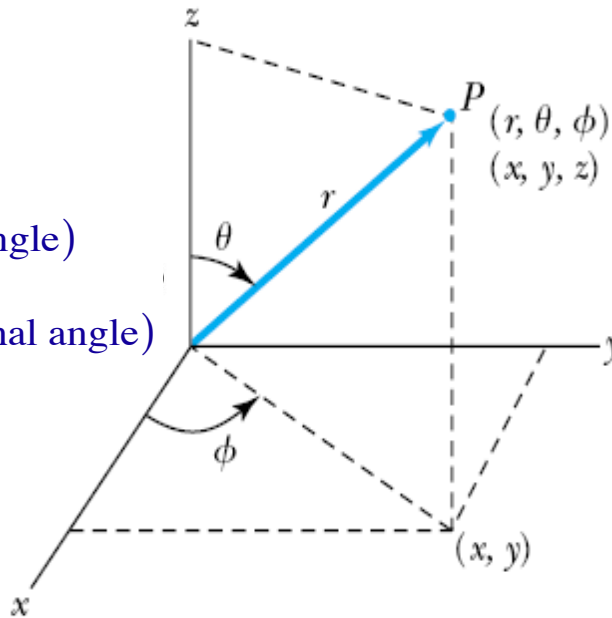
$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

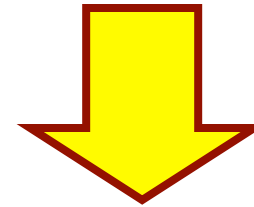
$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \cos^{-1} \frac{z}{r} \text{ (polar angle)}$$

$$\phi = \tan^{-1} \frac{y}{x} \text{ (azimuthal angle)}$$



- Transform to spherical polar coordinates to exploit the radial symmetry.
- Insert the Coulomb potential into the transformed Schrödinger equation.



$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) \psi = 0$$

Application of the Schrödinger Equation

- The wave function ψ is a function of r , θ and ϕ .
 - The equation is separable into three equations of independent variables
 - The solution may be a product of three functions.
 - $$\psi(r, \theta, \phi) = R(r) f(\theta) g(\phi)$$
- We can separate the Schrodinger equation in polar coordinate into three separate differential equations, each depending only on one coordinate: r , θ , or ϕ .

Solution of the Schrödinger Equation for Hydrogen

- Substitute ψ into the polar Schrodinger equation and separate the resulting equation into three equations: $R(r)$, $f(\theta)$, and $g(\phi)$.

Separation of Variables

- The derivatives in Schrodinger eq. can be written as

$$\frac{\partial \psi}{\partial r} = fg \frac{\partial R}{\partial r} \quad \frac{\partial \psi}{\partial \theta} = Rg \frac{\partial f}{\partial \theta} \quad \frac{\partial^2 \psi}{\partial \phi^2} = Rf \frac{\partial^2 g}{\partial \phi^2}$$

- Substituting them into the polar coord. Schrodinger Eq.

$$\frac{fg}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{Rg}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{Rf}{r^2 \sin^2 \theta} \frac{\partial^2 g}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) Rgf = 0$$

- Multiply both sides by $r^2 \sin^2 \theta / Rfg$

$$\frac{\sin^2 \theta}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{\sin \theta}{f} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{g} \frac{\partial^2 g}{\partial \phi^2} + \frac{2\mu}{\hbar^2} r^2 \sin^2 \theta (E - V) = 0$$

Reorganize

$$-\frac{\sin^2 \theta}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{2\mu}{\hbar^2} r^2 \sin^2 \theta (E - V) - \frac{\sin \theta}{f} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) = \frac{1}{g} \frac{\partial^2 g}{\partial \phi^2}$$

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Solution of the Schrödinger Equation

- Only r and θ appear on the left-hand side and only ϕ appears on the right-hand side of the equation
- The left-hand side of the equation cannot change as ϕ changes.
- The right-hand side cannot change with either r or θ .
- Each side needs to be equal to a constant for the equation to be true in all cases. Set the constant $-m_l^2$ equal to the right-hand side of the reorganized equation

$$\frac{d^2 g}{d\phi^2} = -m_l^2 g \quad \text{----- azimuthal equation}$$

– The sign in this equation must be negative for a valid solution

- It is convenient to choose a solution to be $e^{im_l\phi}$.

Solution of the Schrödinger Equation

- $e^{im_l\phi}$ satisfies the previous equation for any value of m_l .
- The solution be single valued in order to have a valid solution for any ϕ , which requires $g(\phi) = g(\phi + 2\pi)$

$$g(\phi = 0) = g(\phi = 2\pi) \quad \Rightarrow \quad e^0 = e^{2\pi im_l}$$

- m_l must be zero or an integer (positive or negative) for this to work
- Now, set the remaining equation equal to $-m_l^2$ and divide either side with $\sin^2\theta$ and rearrange them as

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r^2}{\hbar^2} (E - V) = \frac{m_l^2}{\sin^2 \theta} - \frac{1}{f \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right)$$

- Everything depends on r on the left side and θ on the right side of the equation.