

PHYS 3313 – Section 001

Lecture # 22

Wednesday, April 22, 2015

Dr. Barry Spurlock

- Simple Harmonic Oscillator
- Barriers and Tunneling
- Alpha Particle Decay
- Schrodinger Equation on Hydrogen Atom
- Solutions for Schrodinger Equation for Hydrogen Atom



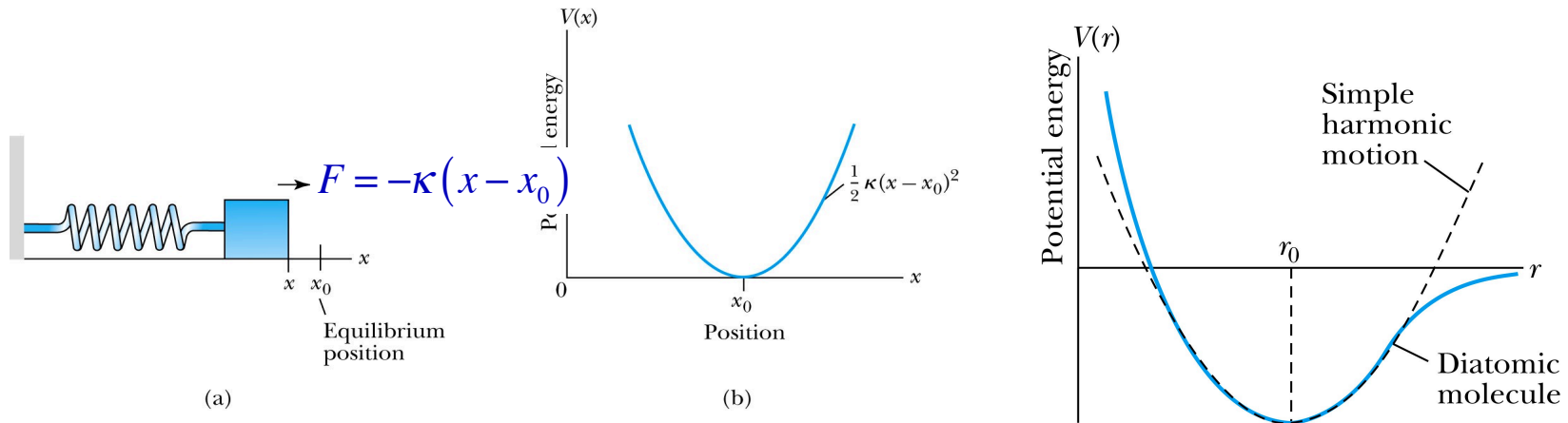
Announcements

- Research paper deadline is Monday, May 4
- Research presentation deadline is Sunday, May 3
- Bring out Homework #5
- Reminder Homework #6
 - CH7 end of chapter problems: 7, 8, 9, 12, 17 and 29
 - Due on Wednesday, Apr. 29, in class
- Reading assignments
 - CH7.6 and the entire CH8
- Quiz number 5
 - At the beginning of the class Wednesday, Apr. 29
 - Covers up to what we finish Monday, Apr. 27



The Simple Harmonic Oscillator

- Simple harmonic oscillators describe many physical situations: springs, diatomic molecules and atomic lattices.



- Consider the Taylor expansion of a potential function:

$$V(x) = V_0 + V_1(x - x_0) + \frac{1}{2} V_2(x - x_0)^2 + \dots$$

The minimum potential at $x = x_0$, so $dV/dx = 0$ and $V_1 = 0$; and the zero potential $V_0 = 0$, we have

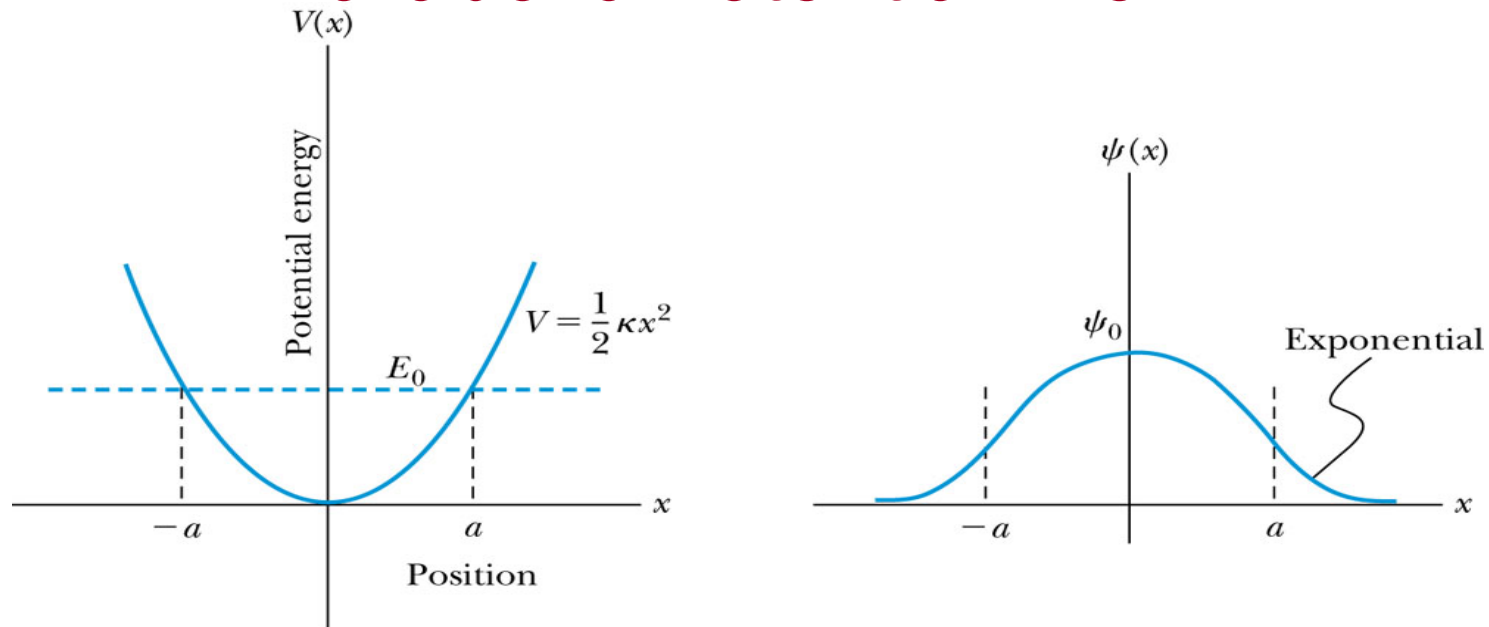
$$V(x) = \frac{1}{2} V_2(x - x_0)^2$$

Substituting this into the wave equation:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \left(E - \frac{\kappa x^2}{2} \right) \psi = \left(-\frac{2m}{\hbar^2} E + \frac{m\kappa x^2}{\hbar^2} \right) \psi$$

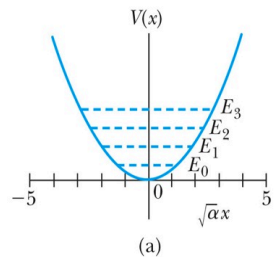
Let $\alpha^2 = \frac{m\kappa}{\hbar^2}$ and $\beta = \frac{2mE}{\hbar^2}$ which yields $\frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta) \psi$.

Parabolic Potential Well



- If the lowest energy level is zero, this violates the uncertainty principle.
- The wave function solutions are $\psi_n = H_n(x) e^{-\alpha x^2/2}$ where $H_n(x)$ are Hermite polynomial function of order n .
- In contrast to the particle in a box, where the oscillatory wave function is a sinusoidal curve, in this case the oscillatory behavior is due to the polynomial, which dominates at small x . The exponential tail is provided by the Gaussian function, which dominates at large x .

Analysis of the Parabolic Potential Well



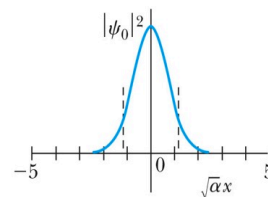
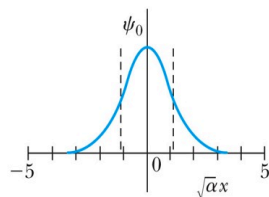
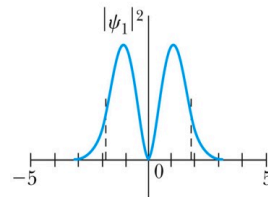
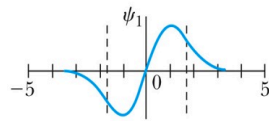
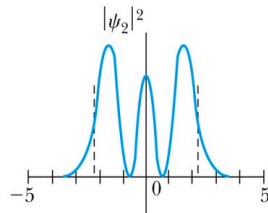
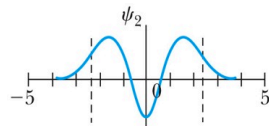
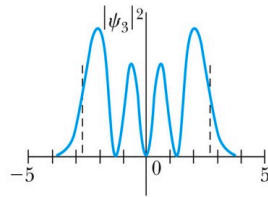
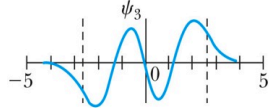
Wave functions

$$\psi_3(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (\sqrt{\alpha}x)(2\alpha x^2 - 3) e^{-\alpha x^2/2}$$

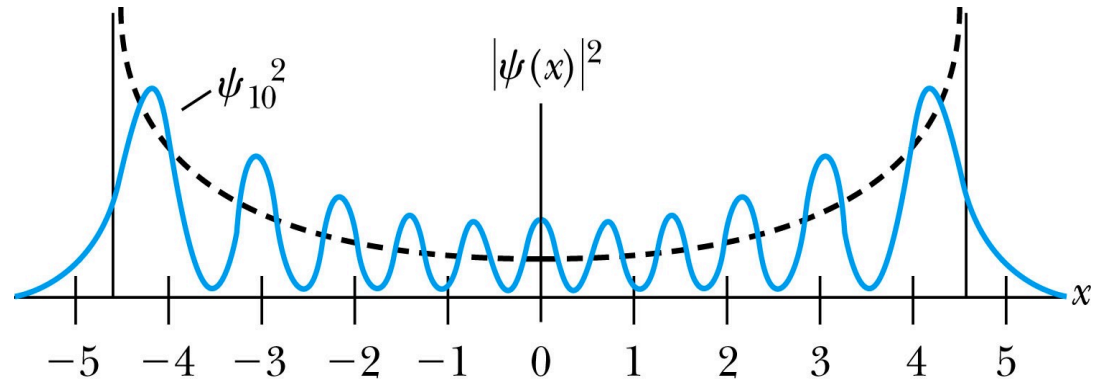
$$\psi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha} x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$



(c)



- The energy levels are given by

$$E_n = \left(n + \frac{1}{2}\right) \hbar \sqrt{\kappa/m} = \left(n + \frac{1}{2}\right) \hbar \omega$$

- The zero point energy is called the Heisenberg limit:

$$E_0 = \frac{1}{2} \hbar \omega$$

- Classically, the probability of finding the mass is greatest at the ends of motion's range and smallest at the center (that is, proportional to the amount of time the mass spends at each position).
- Contrary to the classical one, the largest probability for this lowest energy state is for the particle to be at the center.

Wednesday, April 22,
2015



PHYS 3313-001, Spring 2015
Dr. Jaehoon Yu

Ex. 6.12: Harmonic Oscillator stuff

- Normalize the ground state wave function ψ_0 for the simple harmonic oscillator and find the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$.

$$\psi_n(x) = H_n(x)e^{-\alpha x^2/2} \Rightarrow \psi_0(x) = H_0(x)e^{-\alpha x^2/2} = Ae^{-\alpha x^2/2}$$

$$\int_{-\infty}^{+\infty} \psi_0^* \psi_0 dx = \int_{-\infty}^{+\infty} A^2 e^{-\alpha x^2} dx = 2A^2 \int_0^{+\infty} e^{-\alpha x^2} dx = 2A^2 \left(\frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \right) = 1$$

$$A^2 = \sqrt{\frac{\alpha}{\pi}} \Rightarrow A = \left(\frac{\alpha}{\pi} \right)^{1/4} \Rightarrow H_0(x) = \left(\frac{\alpha}{\pi} \right)^{1/4} \Rightarrow \psi_0(x) = \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2}$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi_0^* x \psi_0 dx = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} x e^{-\alpha x^2} dx = 0$$

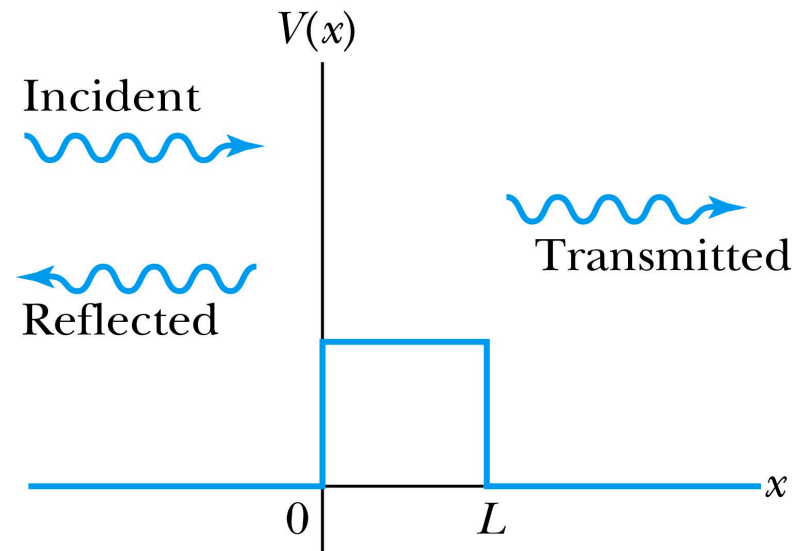
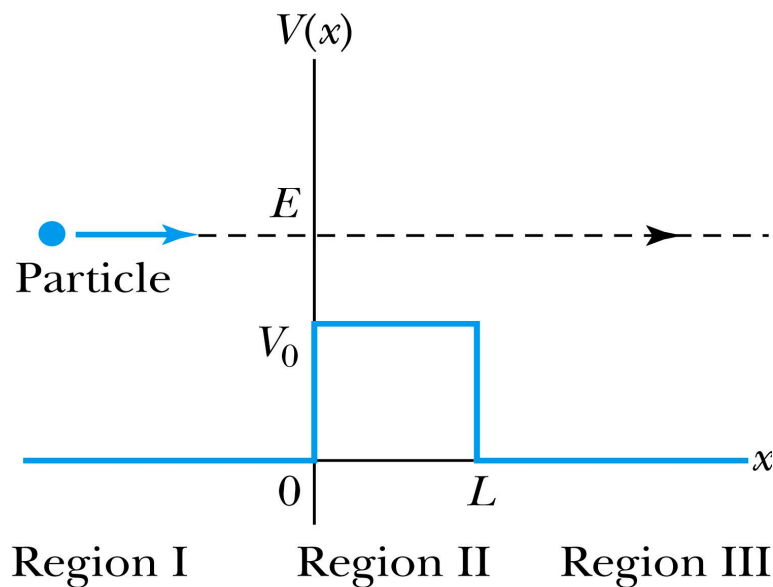
$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} \psi_0^* x^2 \psi_0 dx = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} x^2 e^{-\alpha x^2} dx = 2\sqrt{\frac{\alpha}{\pi}} \int_0^{+\infty} x^2 e^{-\alpha x^2} dx = 2\sqrt{\frac{\alpha}{\pi}} \left(\frac{\sqrt{\pi}}{4\alpha^{3/2}} \right) = \frac{1}{2\alpha}$$

$$\langle x^2 \rangle = \frac{\hbar}{2\sqrt{m\kappa}} \Rightarrow \omega = \sqrt{\kappa/m} \Rightarrow \langle x^2 \rangle = \frac{\hbar}{2m\omega}$$



Barriers and Tunneling

- Consider a particle of energy E approaching a potential barrier of height V_0 and the potential everywhere else is zero.
- We will first consider the case when the energy is greater than the potential barrier.
- In regions I and III the wave numbers are: $k_I = k_{III} = \frac{\sqrt{2mE}}{\hbar}$
- In the barrier region we have $k_{II} = \frac{\sqrt{2m(E - V_0)}}{\hbar}$ where $V = V_0$



Reflection and Transmission

- The wave function will consist of an incident wave, a reflected wave, and a transmitted wave.
- The potentials and the Schrödinger wave equation for the three regions are as follows:

$$\text{Region I } (x < 0) \quad V = 0 \quad \frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2} E \psi_I = 0$$

$$\text{Region II } (0 < x < L) \quad V = V_0 \quad \frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_{II} = 0$$

$$\text{Region III } (x > L) \quad V = 0 \quad \frac{d^2\psi_{III}}{dx^2} + \frac{2m}{\hbar^2} E \psi_{III} = 0$$

- The corresponding solutions are:

$$\text{Region I } (x < 0) \quad \psi_I = Ae^{ik_I x} + Be^{-ik_I x}$$

$$\text{Region II } (0 < x < L) \quad \psi_{II} = Ce^{ik_{II} x} + De^{-ik_{II} x}$$

$$\text{Region III } (x > L) \quad \psi_{III} = Fe^{ik_I x} + Ge^{-ik_I x}$$

- As the wave moves from left to right, we can simplify the wave functions to:

$$\text{Incident wave} \quad \psi_I(\text{incident}) = Ae^{ik_I x}$$

$$\text{Reflected wave} \quad \psi_I(\text{reflected}) = Be^{-ik_I x}$$

$$\text{Transmitted wave} \quad \psi_{III}(\text{transmitted}) = Fe^{ik_I x}$$



Probability of Reflection and Transmission

- The probability of the particles being reflected R or transmitted T is:

$$R = \frac{|\psi_I(\text{reflected})|^2}{|\psi_I(\text{incident})|^2} = \frac{B \cdot B}{A \cdot A}$$

$$T = \frac{|\psi_{III}(\text{transmitted})|^2}{|\psi_I(\text{incident})|^2} = \frac{F \cdot F}{A \cdot A}$$

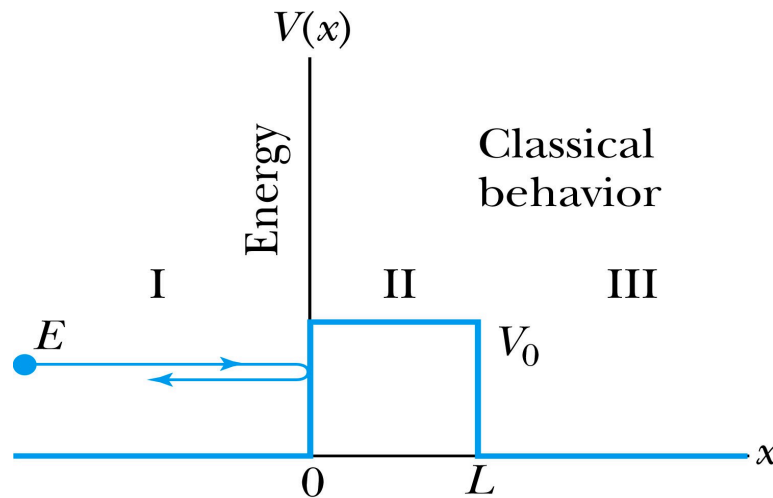
- The maximum kinetic energy of the photoelectrons depends on the value of the light frequency f and not on the intensity.
- Because the particles must be either reflected or transmitted we have: $R + T = 1$
- By applying the boundary conditions $x \rightarrow \pm\infty$, $x = 0$, and $x = L$, we arrive at the transmission probability:

$$T = \left[1 + \frac{V_0^2 \sin^2(k_{II}L)}{4E(E - V_0)} \right]^{-1}$$

- When does the transmission probability become 1?

Tunneling

- Now we consider the situation where classically the particle does not have enough energy to surmount the potential barrier, $E < V_0$.



- The quantum mechanical result, however, is one of the most remarkable features of modern physics, and there is ample experimental proof of its existence. There is a small, but finite, probability that the particle can penetrate the barrier and even emerge on the other side.

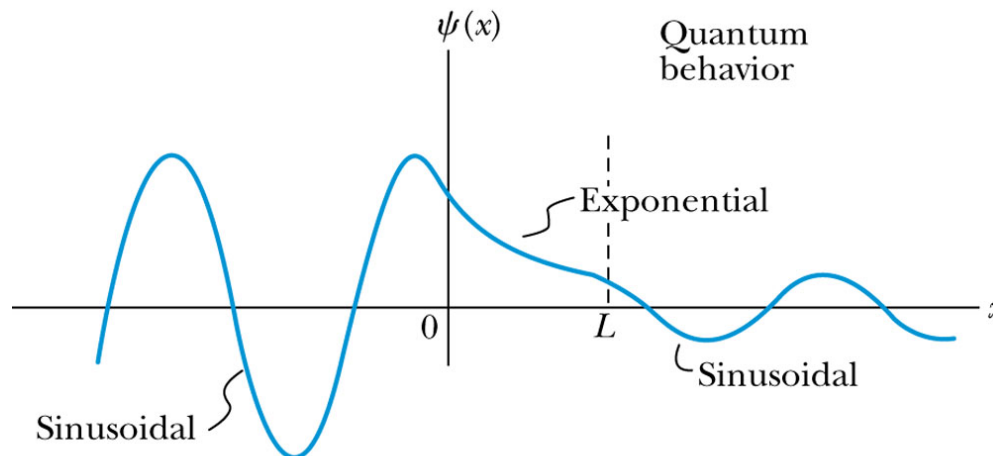
- The wave function in region II becomes $\psi_{II} = Ce^{\kappa x} + De^{-\kappa x}$ where $\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

- The transmission probability that describes the phenomenon of **tunneling** is
$$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa L)}{4E(V_0 - E)} \right]^{-1}$$

Uncertainty Explanation

- Consider when $\kappa L \gg 1$ then the transmission probability becomes:

$$T = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2\kappa L}$$

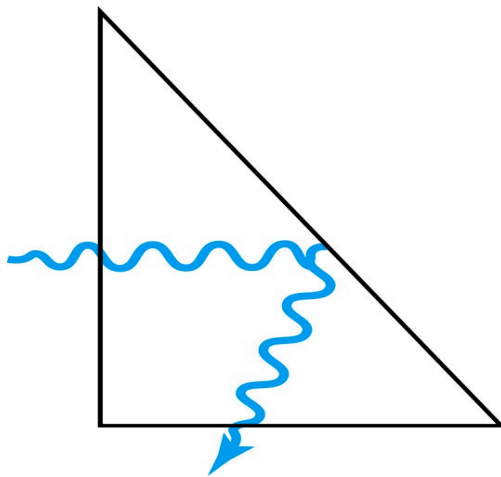


- This violation allowed by the uncertainty principle is equal to the negative kinetic energy required! The particle is allowed by quantum mechanics and the uncertainty principle to penetrate into a classically forbidden region. The minimum such kinetic energy is:

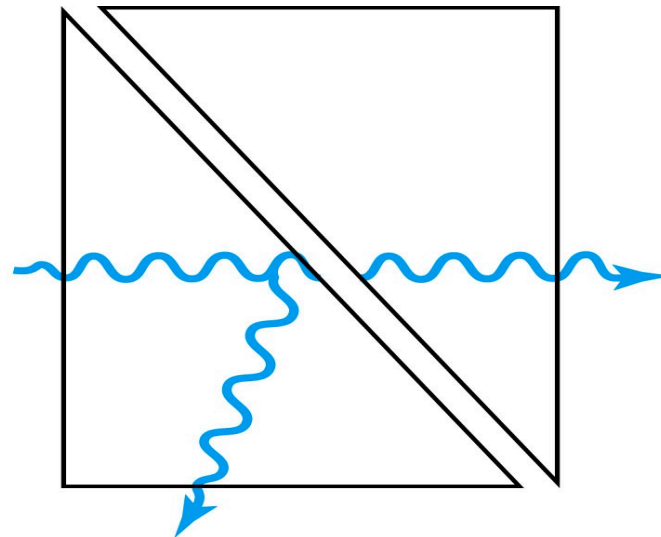
$$K_{\min} = \frac{(\Delta p)^2}{2m} = \frac{\pi^2 \kappa^2}{2m} = V_0 - E$$

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.

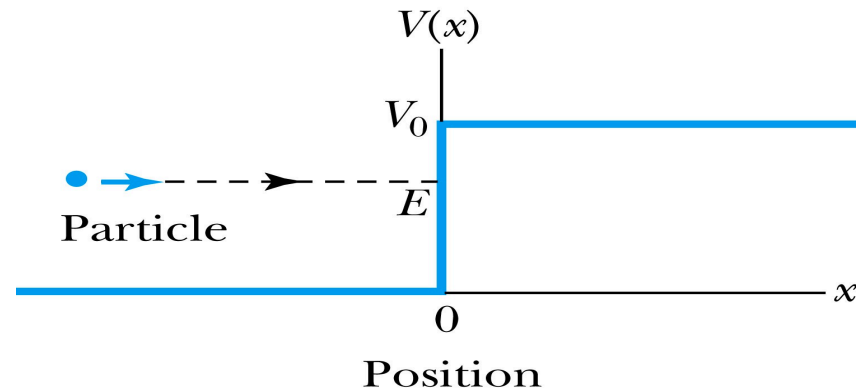


(a)



(b)

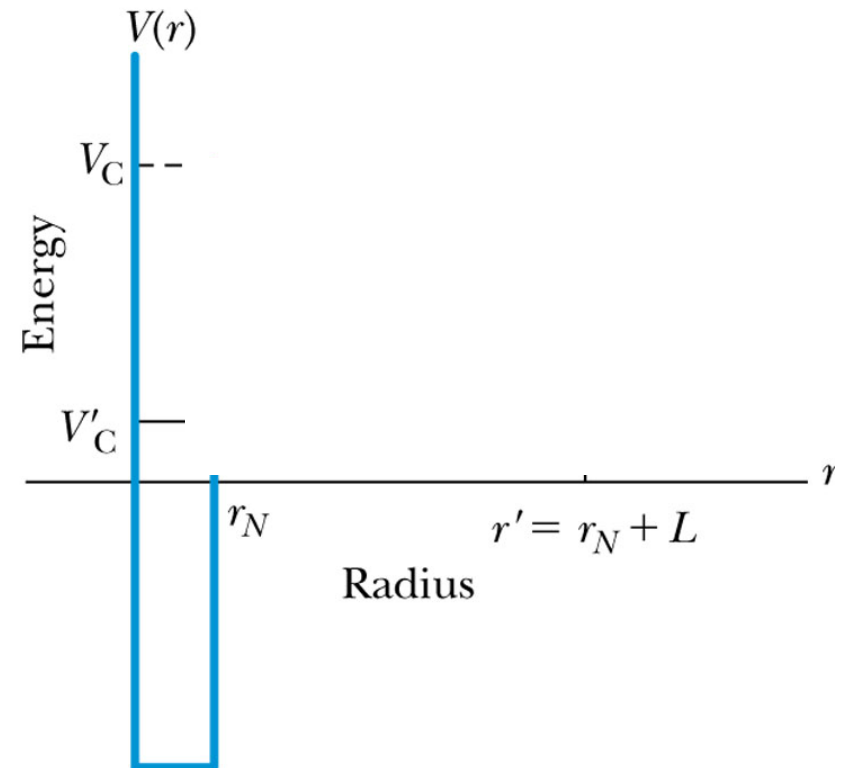
Potential Well



- 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

- May nuclei heavier than Pb emits 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.

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

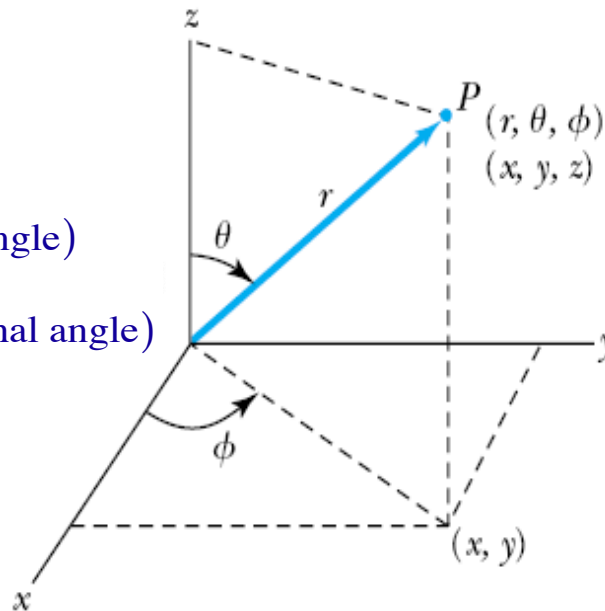
$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

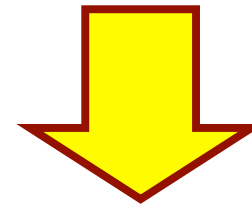
$$r = \sqrt{x^2 + y^2 + z^2}$$

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

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



- 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

- 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 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

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

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.

Solution of the Schrödinger Equation

- Set each side of the equation equal to constant $\ell(\ell + 1)$.

– Radial Equation

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r^2}{\hbar^2} (E - V) = \ell(\ell + 1) \Rightarrow \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E - V - \frac{\hbar^2}{2\mu} \ell(\ell + 1) \right] R = 0$$

– Angular Equation

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \Theta}{\partial \phi^2} = -\ell(\ell + 1) \Rightarrow \frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{df}{d\theta} \right) + \left[\ell(\ell + 1) - \frac{m_l^2}{\sin^2 \theta} \right] f = 0$$

- Schrödinger equation has been separated into three ordinary second-order differential equations, each containing only one variable.

Solution of the Radial Equation

- The radial equation is called the **associated Laguerre equation**, and the *solutions* R that satisfies the appropriate boundary conditions are called *associated Laguerre functions*.
- Assume the ground state has $\ell = 0$, and this requires $m_\ell = 0$.

We obtain

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} [E - V] R = 0$$

- The derivative of $r^2 \frac{dR}{dr}$ yields two terms, and we obtain

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2\mu}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) R = 0$$



Solution of the Radial Equation

- Let's try a solution $R = Ae^{-r/a_0}$ where A is a normalization constant, and a_0 is a constant with the dimension of length.
- Take derivatives of R , we obtain.

$$\left(\frac{1}{a_0^2} + \frac{2\mu}{\hbar^2} E \right) + \left(\frac{2\mu e^2}{4\pi\epsilon_0 \hbar^2} - \frac{2}{a_0} \right) \frac{1}{r} = 0$$

- To satisfy this equation for any r , each of the two expressions in parentheses must be zero.
- Set the second parentheses equal to zero and solve for a_0 .

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2}$$

Bohr's radius

- Set the first parentheses equal to zero and solve for E .

$$E = -\frac{\hbar^2}{2\mu a_0^2} = -E_0 = -13.6 \text{ eV}$$

Ground state energy
of the hydrogen atom

- Both equal to the Bohr's results

Principal Quantum Number n

- The principal quantum number, n , results from the solution of $R(r)$ in the separate Schrodinger Eq. since $R(r)$ includes the potential energy $V(r)$.

The result for this quantized energy is

$$E_n = -\frac{\mu}{2} \left(\frac{e^2}{4\pi\epsilon_0\hbar} \right)^2 \frac{1}{n^2} = -\frac{E_0}{n^2}$$

- The negative sign of the energy E indicates that the electron and proton are bound together.

Quantum Numbers

- The full solution of the radial equation requires an introduction of a quantum number, n , which is a non-zero positive integer.
- The three quantum numbers:
 - n Principal quantum number
 - ℓ Orbital angular momentum quantum number
 - m_ℓ Magnetic quantum number
- The boundary conditions put restrictions on these
 - $n = 1, 2, 3, 4, \dots$ ($n > 0$) Integer
 - $\ell = 0, 1, 2, 3, \dots, n - 1$ ($\ell < n$) Integer
 - $m_\ell = -\ell, -\ell + 1, \dots, 0, 1, \dots, \ell - 1, \ell$ ($|m_\ell| \leq \ell$) Integer
- The predicted energy level is $E_n = -\frac{E_0}{n^2}$



Ex 7.3: Quantum Numbers & Degeneracy

What are the possible quantum numbers for the state $n=4$ in atomic hydrogen? How many degenerate states are there?

n	ℓ	m_ℓ
4	0	0
4	1	-1, 0, +1
4	2	-2, -1, 0, +1, +2
4	3	-3, -2, -1, 0, +1, +2, +3

The energy of a atomic hydrogen state is determined only by the primary quantum number, thus, all these quantum states, $1+3+5+7 = 16$, are in the same energy state.

Thus, there are 16 degenerate states for the state $n=4$.