PHYS 3313 – Section 001
Lecture #15

Monday, Oct. 29, 2012
Dr. Amir Farbin

- Finite Potential Well
- Penetration Depth
- Degeneracy
- Simple Harmonic Oscillator
- Parabolic Potential
- Barriers and Tunneling

Announcements

- Homework #7
  - CH6 end of chapter problems: 34, 39, 46, 62 and 65
  - Due on Monday, Nov. 12, in class
- Quiz #3
  - Beginning of the class Monday, Nov. 12
  - Covers CH5 through what we finish this Wednesday
- Colloquium this week
  - At 4pm, Wednesday, Oct. 31, in SH101

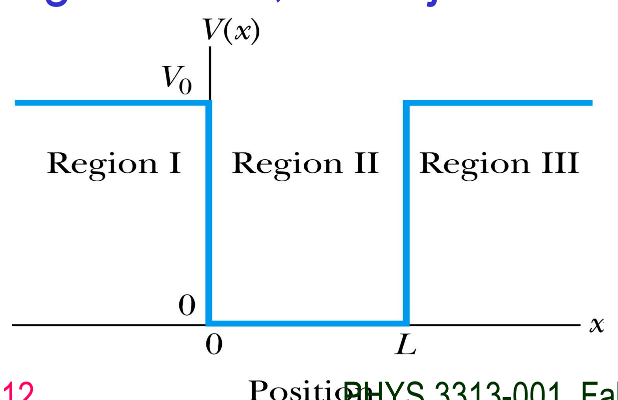
Finite Square-Well Potential

- The finite square-well potential is $$V(x) = \begin{cases} V_0 & x \le 0, \\ 0 & 0 < x < L \\ V_0 & x \ge L \end{cases}$$

- The Schrödinger equation outside the finite well in regions I and III is

$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} = E - V_0$ for regions I and III or using $\alpha^2 = 2m(E - V_0)/\hbar^2$

yields $\frac{d^2\psi}{dx^2} = \alpha^2\psi$. The solution to this differential has exponentials of the form $e^{\alpha x}$ and $e^{-\alpha x}$. In the region x > L, we reject the positive exponential and in the region x < 0, we reject the negative exponential. Why?



$$\psi_I(x) = Ae^{\alpha x} \quad \text{region I}, x < 0$$
$$\psi_{III}(x) = Ae^{-\alpha x} \quad \text{region III}, x > L$$

This is because the wave function should be 0 as x→infinity.

Finite Square-Well Solution

- Inside the square well, where the potential *V* is zero and the particle is free, the wave equation becomes $\frac{d^2\psi}{dx^2} = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$
- Instead of a sinusoidal solution we can write

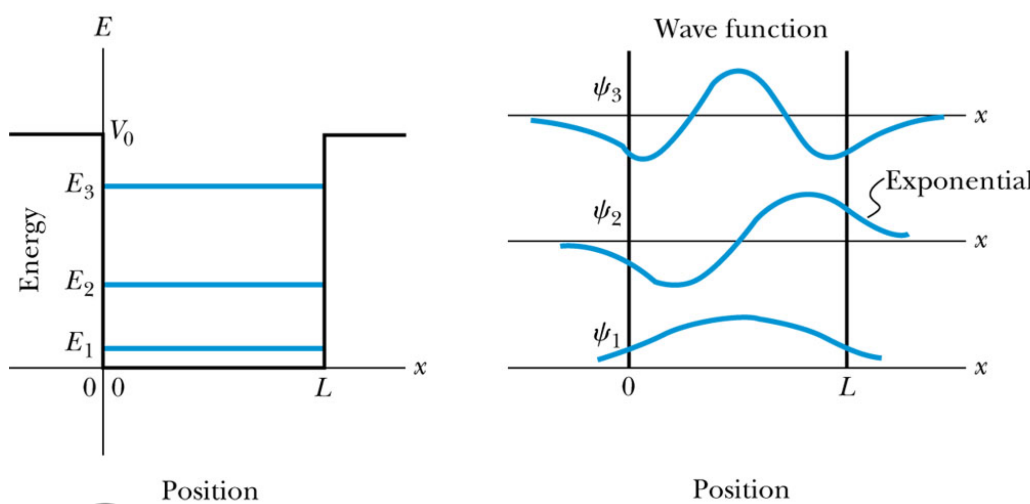
$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx} \quad \text{region II, } 0 < x < L$$

- The boundary conditions require that

$$\psi_I = \psi_{II} \text{ at } x = 0 \text{ and } \psi_I = \psi_{III} \text{ at } x = L$$

and the wave function must be smooth where the regions meet.

- Note that the wave function is nonzero outside of the box.
- Non-zero at the boundary either..
- What would the energy look like?



Penetration Depth

- The penetration depth is the distance outside the potential well where the probability significantly decreases. It is given by

$$\delta x \approx \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(E - V_0)}}$$

- It should not be surprising to find that the penetration distance that violates classical physics is proportional to Planck's constant.

Three-Dimensional Infinite-Potential Well

- The wave function must be a function of all three spatial coordinates.

  We begin with the conservation of energy $E = K + V = \frac{p^2}{2m} + V$

- Multiply this by the wave function to get

$$E\psi = \left(\frac{p^2}{2m} + V\right)\psi = \frac{p^2}{2m}\psi + V\psi$$

- Now consider momentum as an operator acting on the wave function. In this case, the operator must act twice on each dimension. Given:

$$p^2 = p_x^2 + p_y^2 + p_z^2 \qquad \hat{p}_x\psi = -i\hbar\frac{\partial\psi}{\partial x} \quad \hat{p}_y\psi = -i\hbar\frac{\partial\psi}{\partial y} \quad \hat{p}_z\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

- The three dimensional Schrödinger wave equation is

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

Rewrite ⇒

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

Ex 6.10: Expectation values inside a box

Consider a free particle inside a box with lengths L_1, L_2 and L_3 along the x, y, and z axes, respectively, as shown in Fire. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the round energy and wave function and the energy of the first excited state for a cube of sides L.

What are the boundary conditions for this situation?

Particle is free, so x, y and z wave functions are independent from each other!

Each wave function must be 0 at the wall! Inside the box, potential V is 0.

$$-\frac{\hbar}{2m}\nabla^2\psi + V\psi = E\psi \Rightarrow -\frac{\hbar}{2m}\nabla^2\psi = E\psi$$

A reasonable solution is

$$\psi(x,y,z) = A\sin(k_1 x)\sin(k_2 y)\sin(k_3 z)$$

Using the boundary condition

$$\psi = 0 \text{ at } x = L_1 \Rightarrow k_1 L_1 = n_1\pi \Rightarrow k_1 = n_1\pi / L_1$$

So the wave numbers are $k_1 = \frac{n_1\pi}{L_1}$ $\quad k_2 = \frac{n_2\pi}{L_2}$ $\quad k_3 = \frac{n_3\pi}{L_3}$

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The energy can be obtained through the Schrodinger equation

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

$$\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = k_1A\cos(k_1x)\sin(k_2y)\sin(k_3z)$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2}{\partial x^2}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = -k_1^2A\sin(k_1x)\sin(k_2y)\sin(k_3z) = -k_1^2\psi$$

$$-\frac{\hbar}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right)\psi = E\psi$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right) = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2}+\frac{n_2^2}{L_2^2}+\frac{n_3^2}{L_3^2}\right)$$

What is the ground state energy?

$E_{1,1,1}$ when $n_1=n_2=n_3=1$, how much?

When are the energies the same for different combinations of n_i?

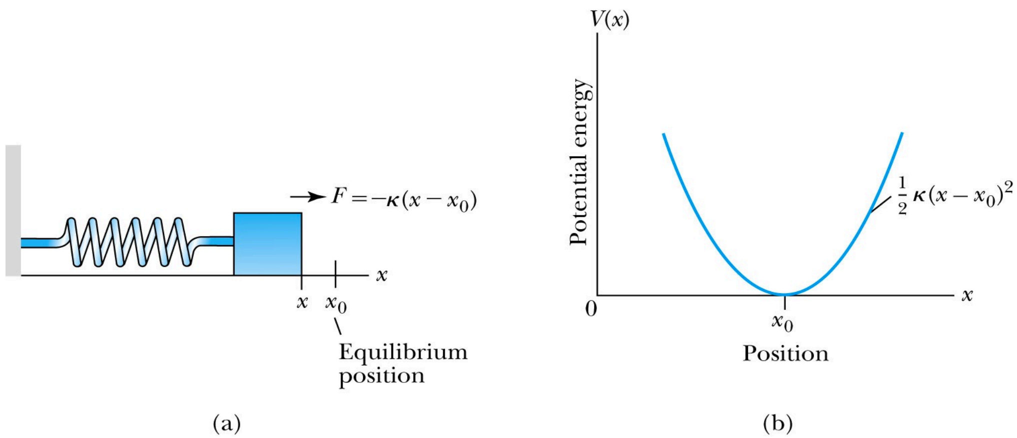
Degeneracy*

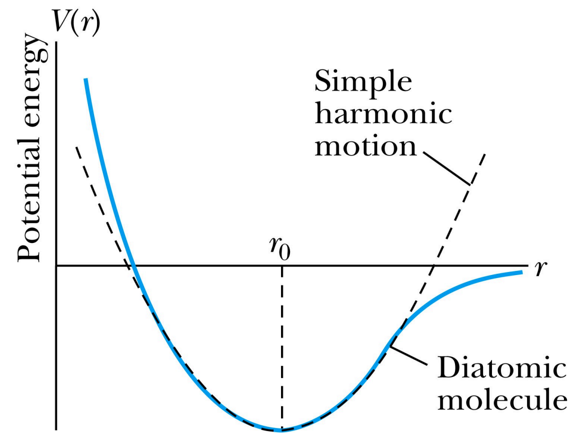
- Analysis of the Schrödinger wave equation in three dimensions introduces three quantum numbers that quantize the energy.
- A quantum state is degenerate when there is more than one wave function for a given energy.
- Degeneracy results from particular properties of the potential energy function that describes the system. A perturbation of the potential energy, such as spin under a B field, can remove the degeneracy.

***Mirriam-webster: having two or more states or subdivisions having two or more states or subdivisions**

Simple Harmonic Oscillator

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





- Consider the Taylor expansion of a potential function:

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

Redefining the minimum potential and the zero potential, we have

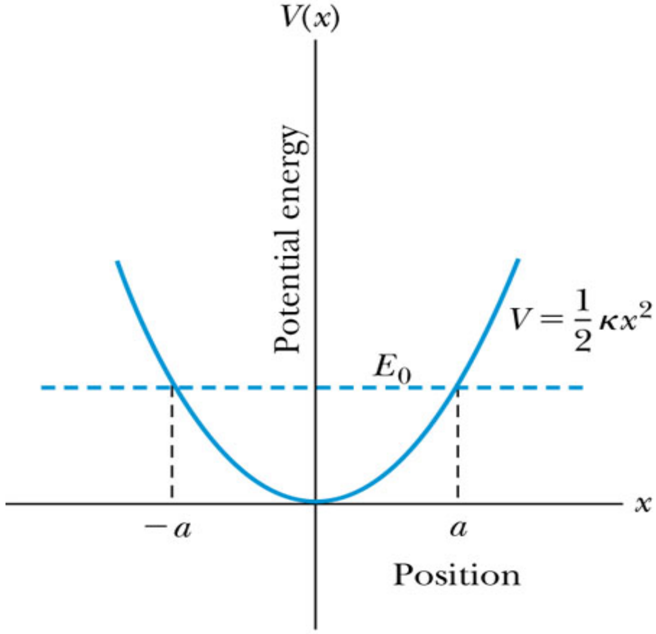
$$V(x) = \frac{1}{2}V_2(x - x_0)^2$$

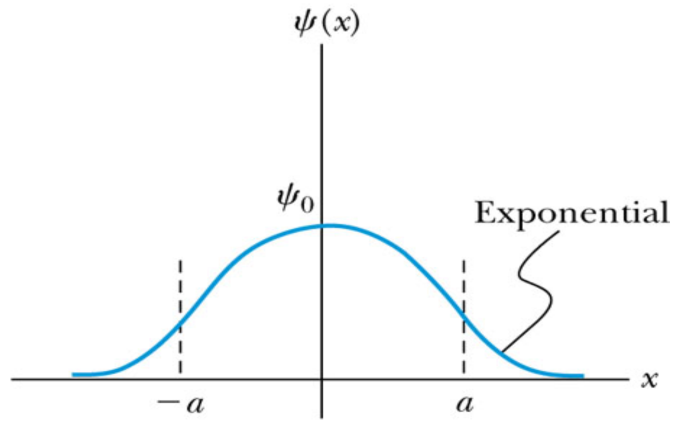
Substituting this into the wave equation:

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

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

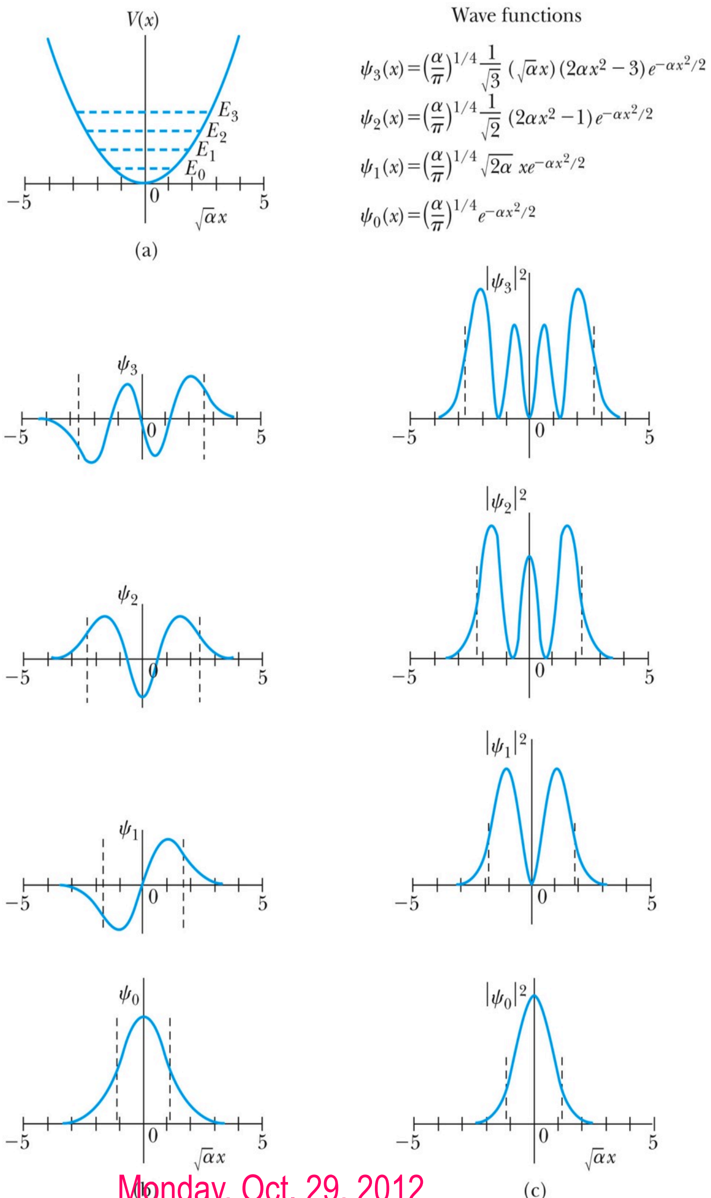
Parabolic Potential Well

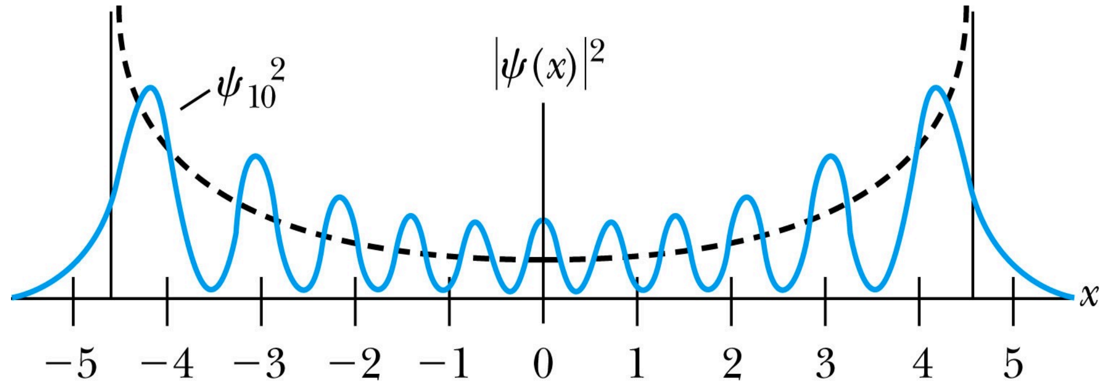




- If the lowest energy level is zero, this violates the uncertainty principle.
- The wave function solutions are $\psi_n = H_n(x)e^{-\alpha x^2/2}$ where $H_n(x)$ are Hermite polynomials of order *n*.
- In contrast to the particle in a box, where the oscillatory wave function is a sinusoidal curve, in 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





- The energy levels are given by

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

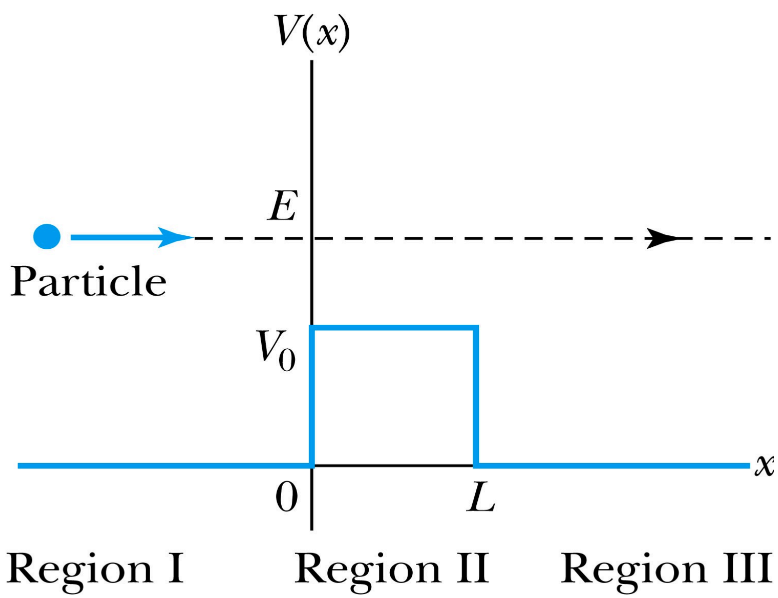
- The zero point energy is called the Heisenberg limit:

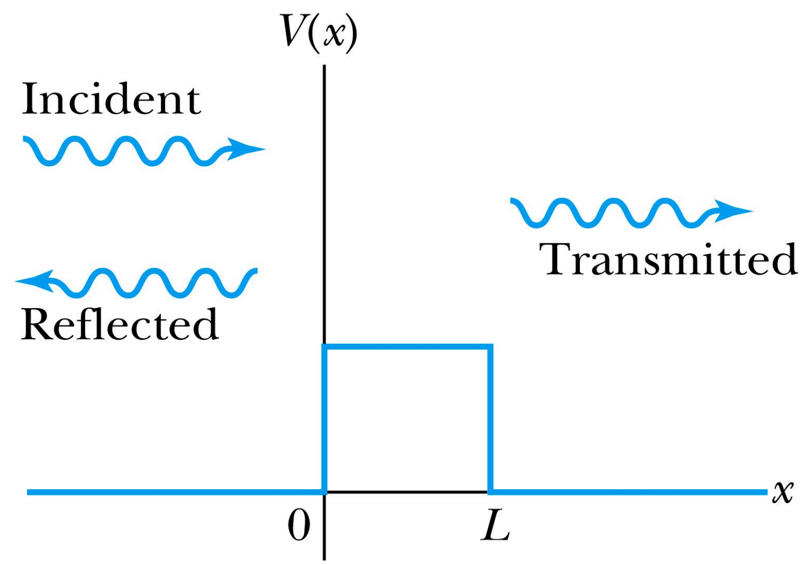
$$E_0 = \frac{1}{2}\hbar\omega$$

- Classically, the probability of finding the mass is greatest at the ends of motion 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.

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 $$k_{II} = \frac{\sqrt{2m(E - V_0)}}{\hbar} \quad \text{where } V = V_0$$





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:

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

- The corresponding solutions are:

Region I ($x < 0$)	$\psi_I = Ae^{ik_I x} + Be^{-ik_I x}$
Region II ($0 < x < L$)	$\psi_{II} = Ce^{ik_{II} x} + De^{-ik_{II} x}$
Region III ($x > L$)	$\psi_{III} = Fe^{ik_I x} + Ge^{-ik_I x}$

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

Incident wave	$\psi_I(\text{incident}) = Ae^{ik_I x}$
Reflected wave	$\psi_I(\text{reflected}) = Be^{-ik_I x}$
Transmitted wave	$\psi_{III}(\text{transmitted}) = Fe^{ik_I x}$

Probability of Reflection and Transmission

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

$$R = \frac{|\psi_{\mathrm{I}}(\text{reflected})|^2}{|\psi_{\mathrm{I}}(\text{incident})|^2} = \frac{B^* B}{A^* A}$$

$$T = \frac{|\psi_{\mathrm{III}}(\text{transmitted})|^2}{|\psi_{\mathrm{I}}(\text{incident})|^2} = \frac{F^* F}{A^* A}$$

- 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 $x \to \pm\infty$, $x = 0$, and $x = L$, we arrive at the transmission probability:

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

- Notice that there is a situation in which the transmission probability is 1.