PHYS 3313 – Section 001
Lecture #21

Wednesday, April 10, 2019
Dr. Jaehoon Yu

- Simple Harmonic Oscillator
- Reflection and Transmission
- Barriers and Tunneling
- Alpha Particle Decay
- Schrodinger Equations applied on Hydrogen Atom

Announcements

- Reminder: Homework #5
  - CH6 end of chapter problems: 34, 46 and 65
  - CH7 end of chapter problems: 7, 9, 17 and 29
  - Due Monday, Apr. 15
- Quiz #4 coming Monday, Apr. 15
  - Beginning of the class; Covers CH6.2 to the end of CH 6
  - BYOF: You may bring a one 8.5x11.5 sheet (front and back) of handwritten formulae and values of constants for the exam
- Quiz 3 results
  - Class average: 34.3/50
    - Equivalent to 68.6/100
    - Previous results: 37.2 and 56.2
  - Class top score: 50/50
- Colloquium 4pm today in SH101
  - Dr. V. Chirayath of UTA

Physics Department
The University of Texas at Arlington
COLLOQUIUM

Positron annihilation spectroscopy: A novel method to investigate 2D materials and internal surfaces

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University of Texas at Arlington

Wednesday April 10, 2019
4:00 p.m. Room 101 Science Hall

Abstract

The electronic structure and the chemical architecture of external/internal surfaces and buried interfaces determine the efficiency of various catalytic processes as well as the performance of hetero-structured devices. Researchers employ novel techniques to probe the top atomic layers of the external and internal surfaces or buried interfaces with minimal contribution from the underlying bulk. Surface spectroscopy using positrons stand out among these techniques because of its ability to sample only the top few mono-layers resulting in signals that is sensitive to the surface electronic density of states and the surface chemical composition. The surface selectivity of positrons stem from the trapping of positrons in an image-potential induced surface state before its annihilation with the surface electrons. The interaction of the positron with the surface electrons results in two signals which can be used to extract the surface electronic and chemical composition, (a) the annihilation gamma photon and (b) the Auger electron emission initiated by the hole created by the annihilation process. We have employed the mono-layer selectivity of positrons to measure the positron annihilation induced Auger electron spectrum (PAES) from single layer graphene (SLG) deposited on a copper (Cu) substrate. The electron spectrum revealed the presence of an Auger emission process starting from the valence band of graphene that has not been observed previously in spite of the theoretical prediction of its existence. I will discuss the importance of this process, termed as "VVV" in the first section of the presentation. The Doppler broadening of the annihilation gamma has been used extensively to derive chemical and defect information from the bulk and the sub-surface regions. However, there are few studies using Doppler broadening spectroscopy to derive chemical information from top one or two atomic layers. Our investigation on graphene on Cu has shown us that the Doppler broadening spectroscopy carries distinct signature of the chemical composition of the top surface. This prompted us to propose a novel technique using positrons to probe the inner-hidden surfaces of porous materials. Few techniques can directly probe the inner surfaces of porous materials as the electron or low energy photon signal generated from the inner surfaces cannot escape from the sample. The ability of the positrons to trap at surface state combined with the ability of a 511 keV annihilation gamma to traverse through the sample and the ultra high vacuum chamber is utilised in this method to characterize the inner surface chemical composition. In the second section of the presentation, I will discuss the developments of this novel technique at our newly developed advanced positron beam at UTA.

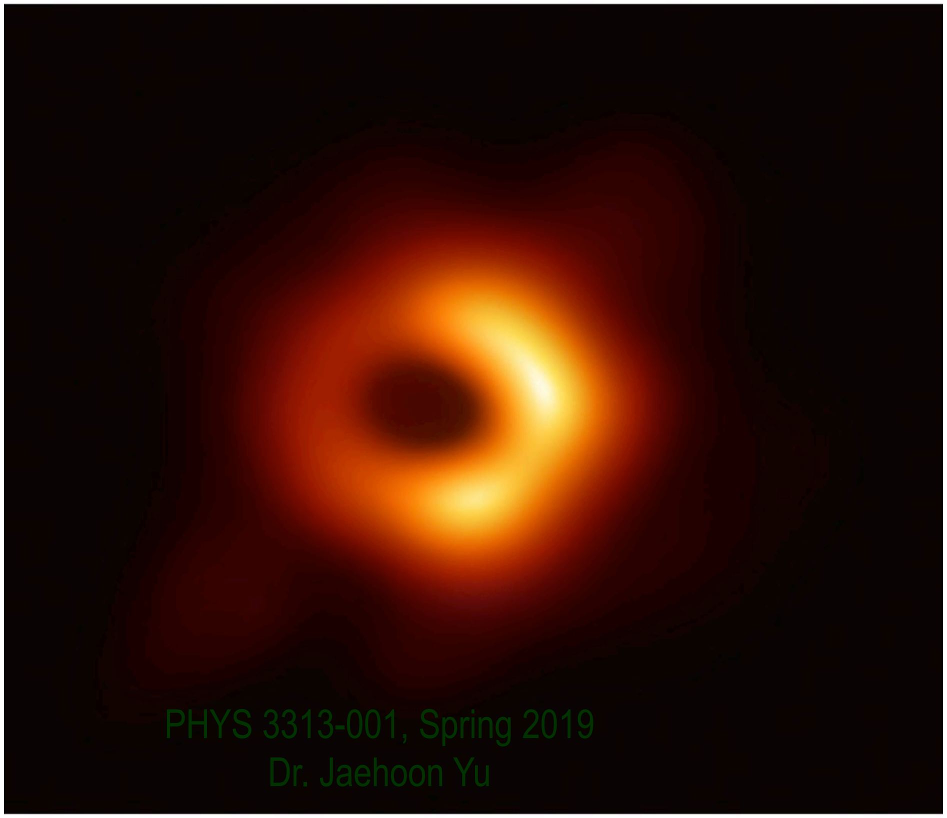
Refreshments will be served at 3:30 p.m. in the Physics Lounge

Reminder: Special Project #7

- Show that the Schrodinger wave equation becomes Newton's second law in the classical limit. (15 points)
- Deadline Wednesday, Apr. 17
- You MUST have your own answers!

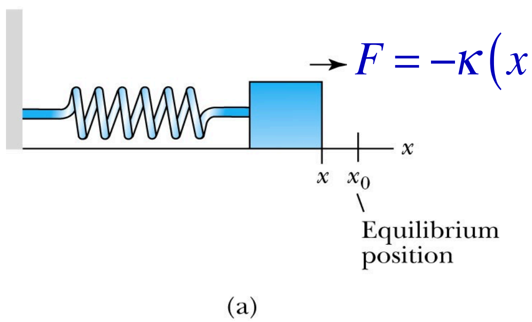
The Black Hole Observation

- Announced today by the Event Horizon Telescope (EHT) Collaboration
- First positive confirmation of the existence of the Black Hole predicted by Einstein's general relativity in 1915

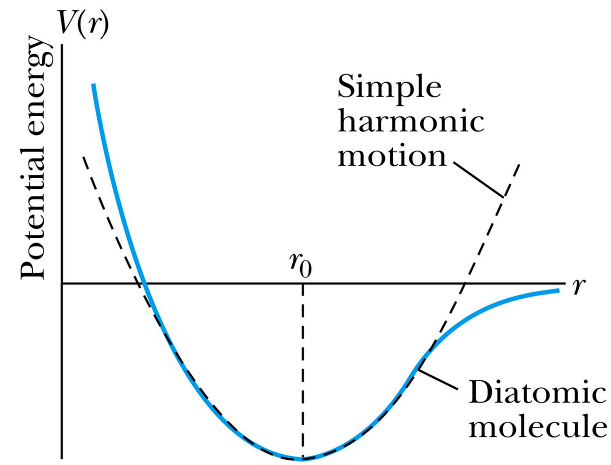


The Simple Harmonic Oscillator

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



$$F = -\kappa(x - x_0)$$



- Consider the Taylor expansion of a potential function:

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

The minimum potential at $x=x_0$, $dV/dx=0$ ➔ $V_1=0$ and the zero potential $V_0=0$, then we have the potential of the form

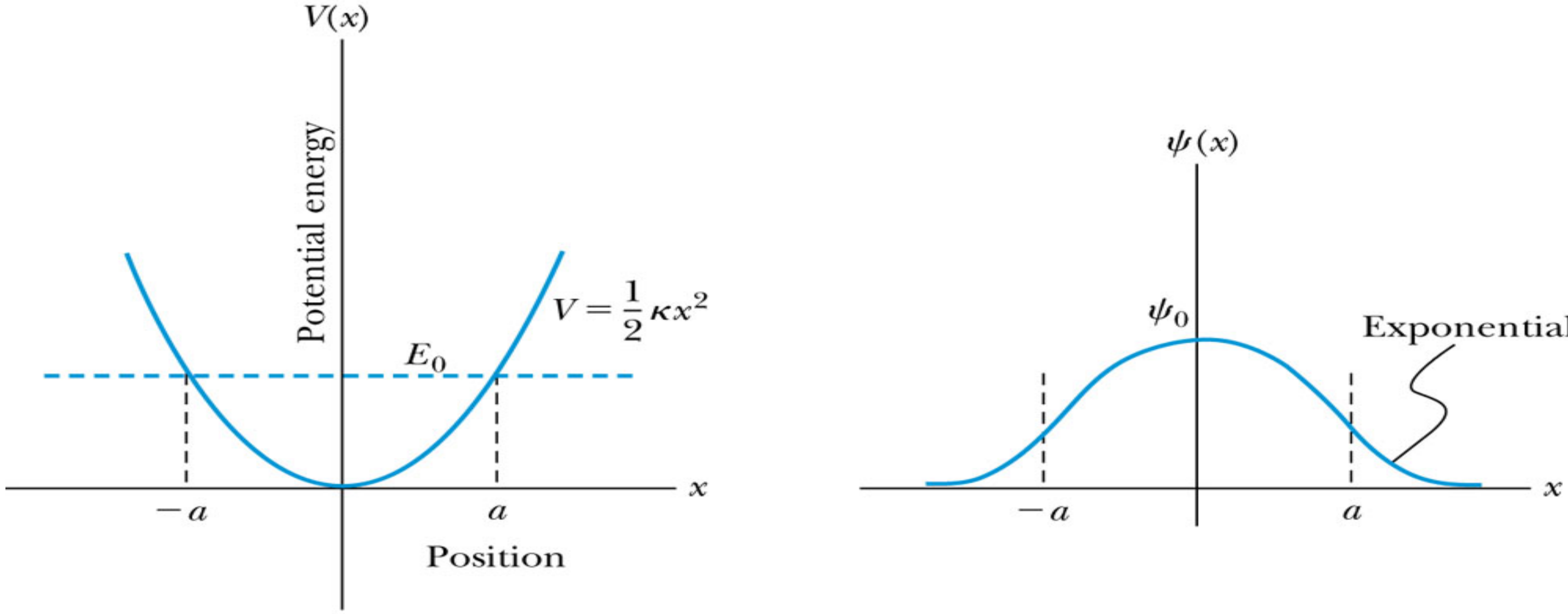
$$V(x) = \frac{1}{2}V_2(x - x_0)^2$$

Substituting this into the wave equation (make $x_0=0$):

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

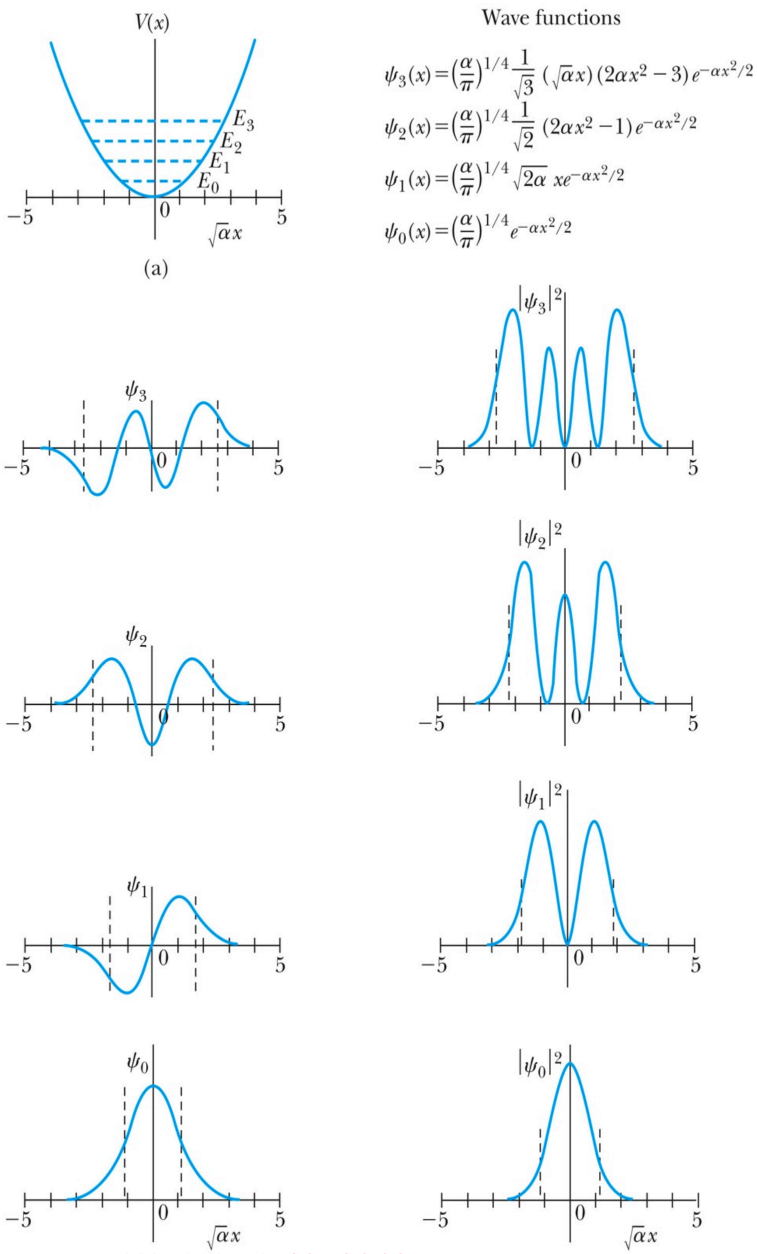
Let $\alpha^2 = \frac{m\kappa}{\hbar^2}$ and $\beta = \frac{2mE}{\hbar^2}$ which yields $\frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta)\psi$.

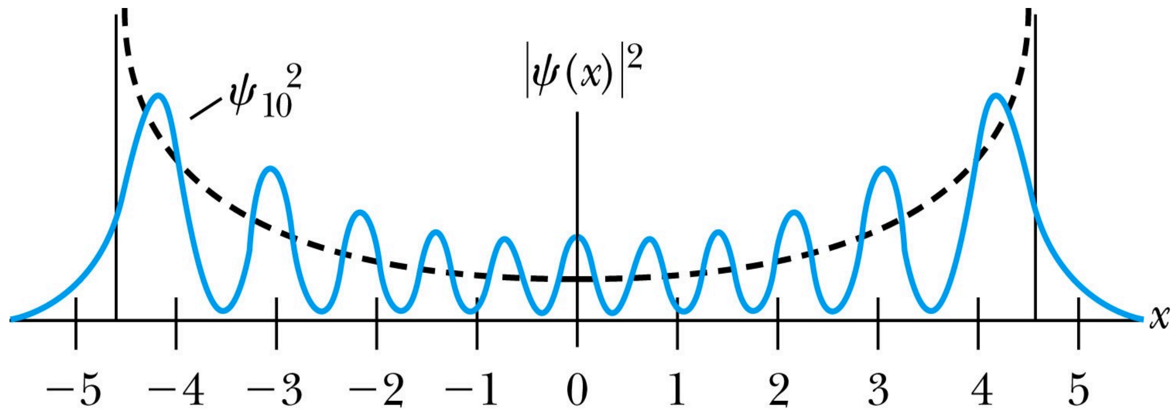
Parabolic Potential Well



- If the lowest energy level is zero, this violates the uncertainty principle since both x and p must be 0 at the same time.➔ So E cannot be 0!
- 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 (H_n) 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'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.

Ex. 6.12: Harmonic Oscillator stuff

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

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

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

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

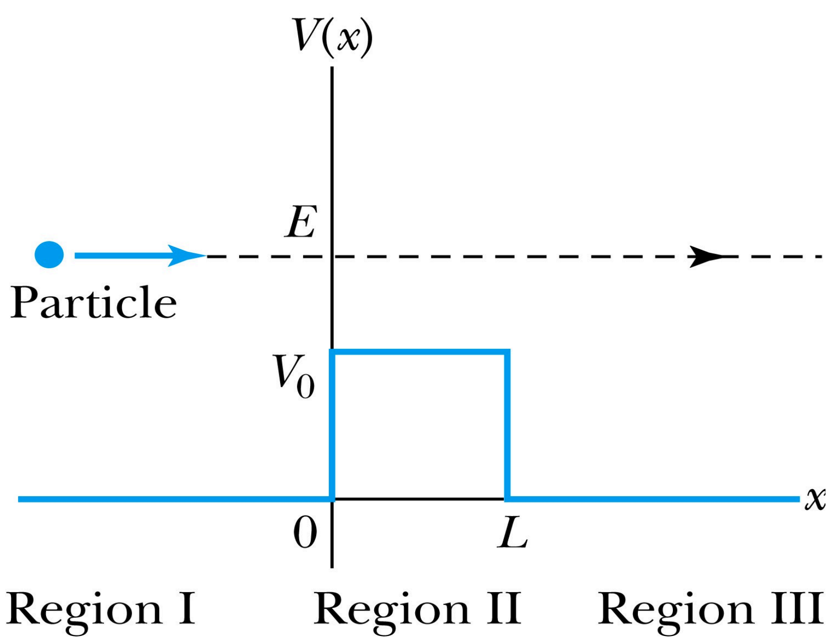
$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi_0^* x \psi_0 \, dx = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} x e^{-\alpha x^2} \, dx = 0$$

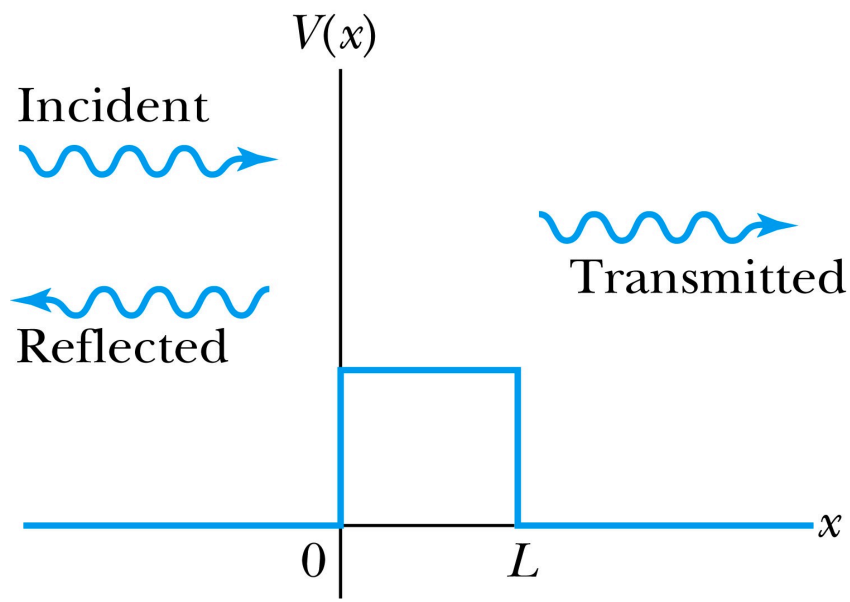
$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} \psi_0^* x^2 \psi_0 \, dx = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} x^2 e^{-\alpha x^2} \, dx = 2\sqrt{\frac{\alpha}{\pi}} \int_0^{+\infty} x^2 e^{-\alpha x^2} \, dx = 2\sqrt{\frac{\alpha}{\pi}} \left(\frac{\sqrt{\pi}}{4\alpha^{3/2}} \right)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

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

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





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:

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

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

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

- The corresponding solutions are:

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

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

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

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

$$\text{Incident wave} \qquad \psi_I(\text{incident})=Ae^{ik_Ix}$$

$$\text{Reflected wave} \qquad \psi_I(\text{reflected})=Be^{-ik_Ix}$$

$$\text{Transmitted wave} \qquad \psi_{III}(\text{transmitted})=Fe^{ik_Ix}$$

Probability of Reflection and Transmission

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

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

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

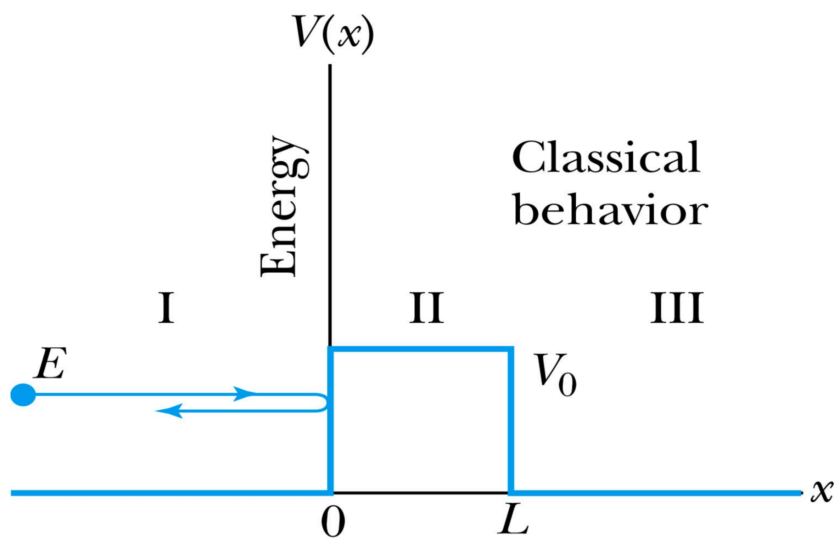
- The maximum kinetic energy of the photoelectrons depends on the value of the light frequency *f* and not on the intensity.
- Because the particles must be either reflected or transmitted we have: $R + T = 1$
- By applying the boundary conditions $x \to \pm\infty$, $x = 0$, and $x = L$, we arrive at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

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

- 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*$_0$**.

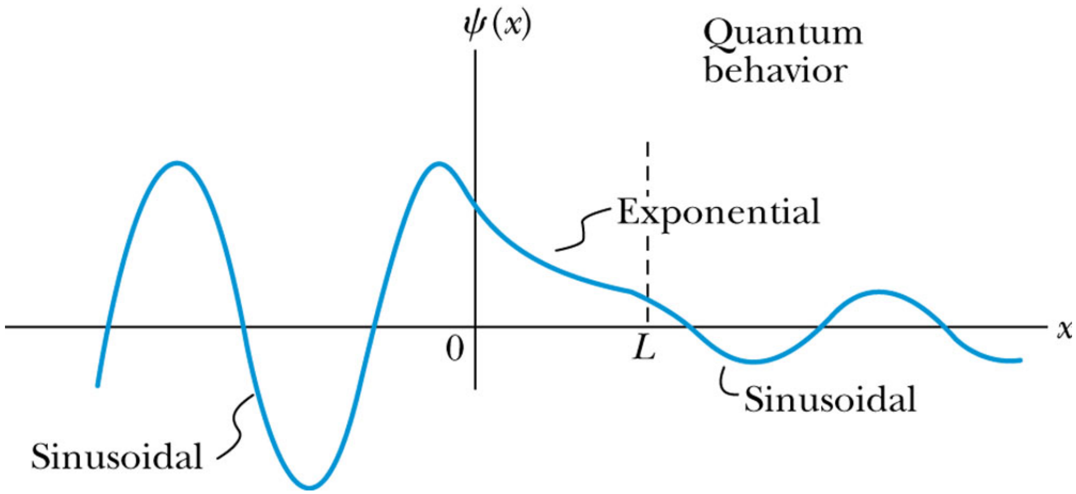


- The quantum mechanical result, however, is one of the most remarkable features of modern physics, and there is ample experimental proof of its existence. There is a small, but finite, probability that the particle can penetrate the barrier and even emerge on the other side.
- The wave function in region II becomes $$\psi_{II} = Ce^{\kappa x} + De^{-\kappa x} \quad \text{where } \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$
- 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 κL >> 1 then the transmission probability becomes:

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

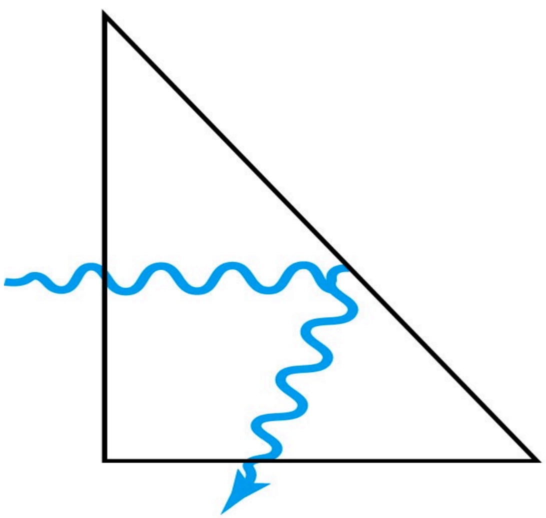


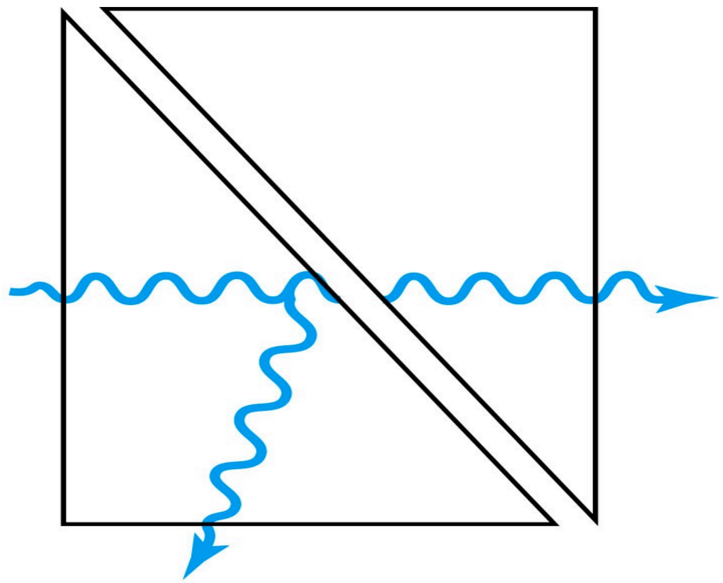
- This violation allowed by the uncertainty principle is equal to the negative kinetic energy required! The particle is allowed by quantum mechanics and the uncertainty principle to penetrate into a classically forbidden region. The minimum such kinetic energy is:

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

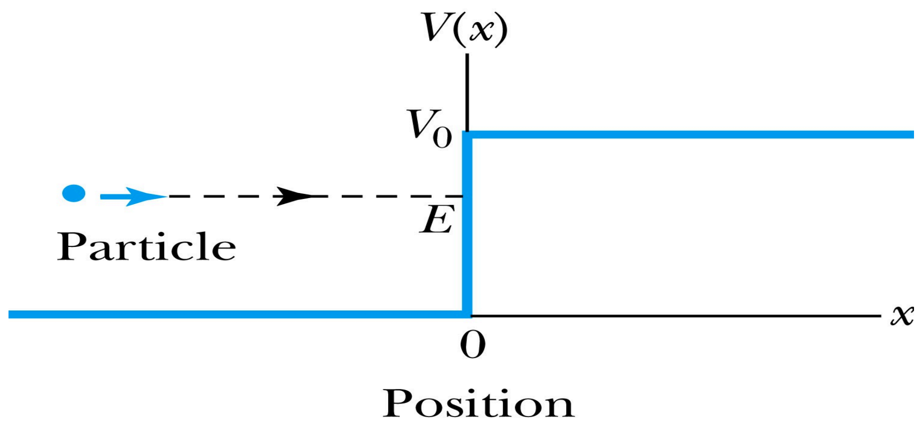
Analogy with Wave Optics

- 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

- Many 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 (~5MeV).
- According to quantum mechanics, however, the alpha particle can "tunnel" through the barrier. Hence this is observed as radioactive decay.