PH 112: Quantum Physics and Applications

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Week 05 Lecture 03: Finite Step Potential

D3, Spring 2023

Fourth Application: Step Potential (Recap)

- A quantum particle that is incident on a finite potential barrier may cross the barrier.

- It does not have a classical analog.

- Penetration depth is $$\delta x \simeq \frac{1}{k_{II}} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Fifth Application: Finite Step potential

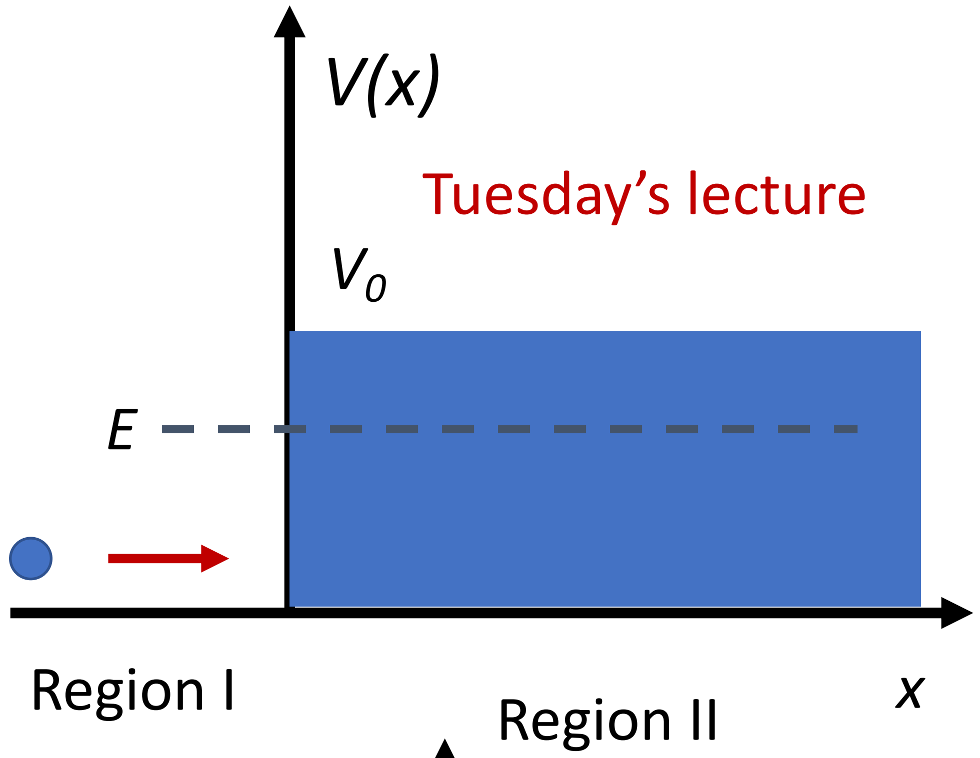
Potential Barrier

- A potential barrier is the opposite of Potential well.

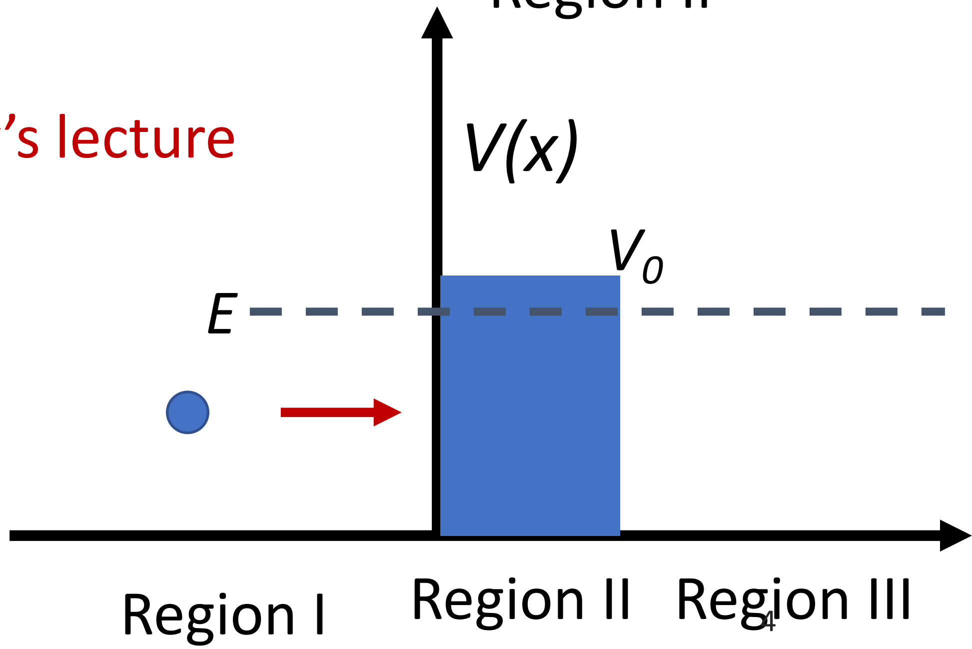
- Consider a flux of particles incident from the left on the potential step or barrier with energy E. We assume there is no flux of particles coming from the right.

- Region I and III: Kinetic Energy: E

- Region II: Kinetic energy: $E - V_0$



Today's lecture



Finite Potential Barrier: Classical

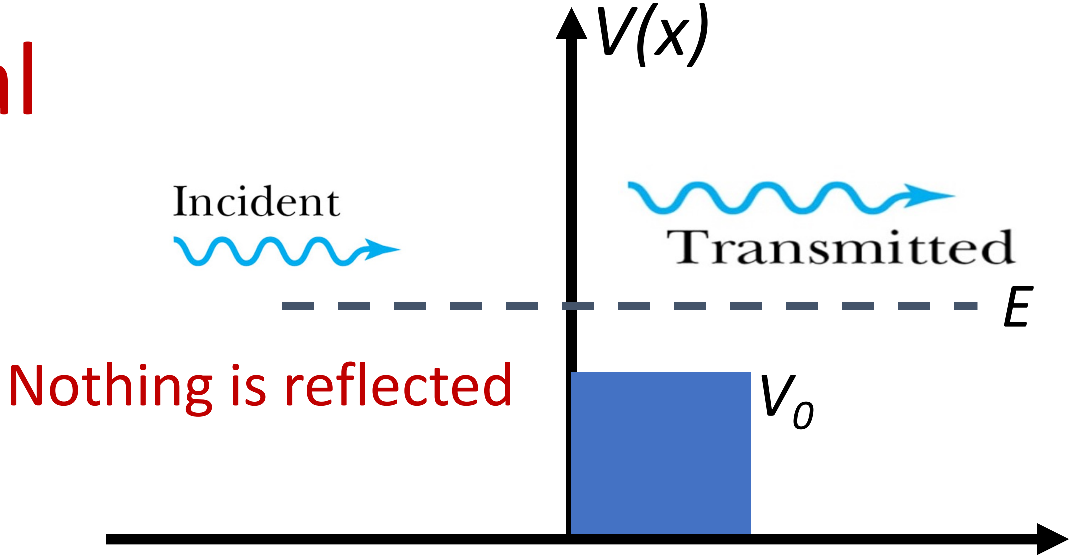
- For $E > V_0$:

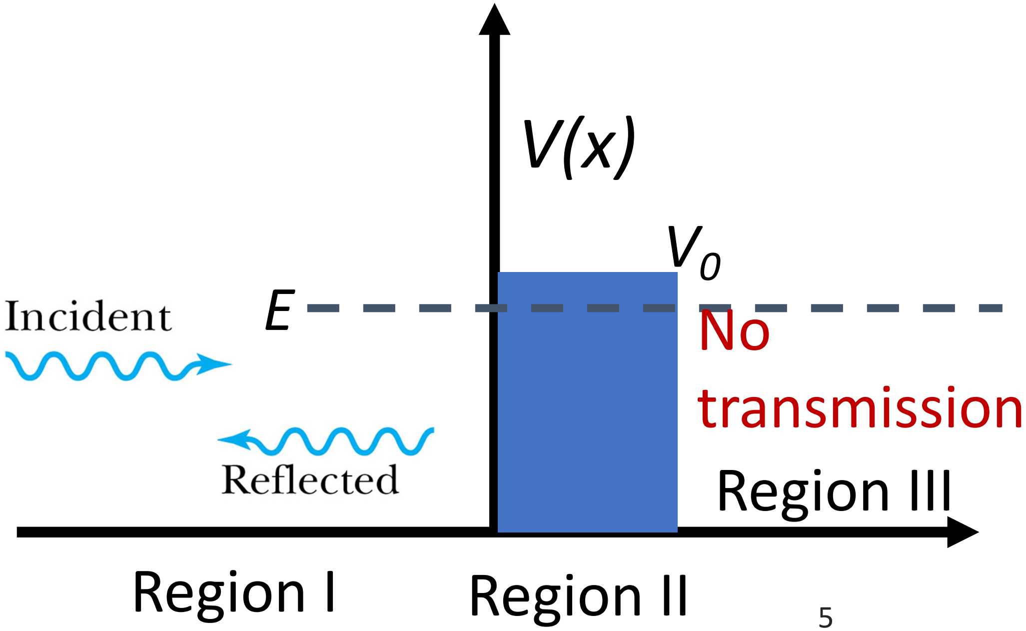
  1. all the particles will pass over the step/barrier (they are transmitted).

  2. the particles will slow down (smaller momentum).

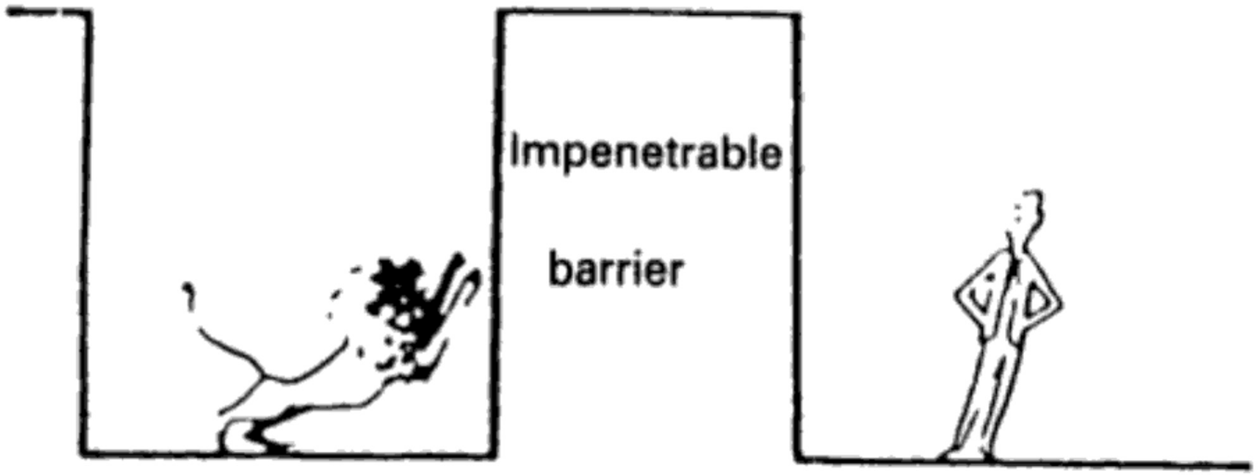
- For $E < V_0$: all the particles are reflected!

The flux of particles are the same. (There is no source or sink anywhere.)

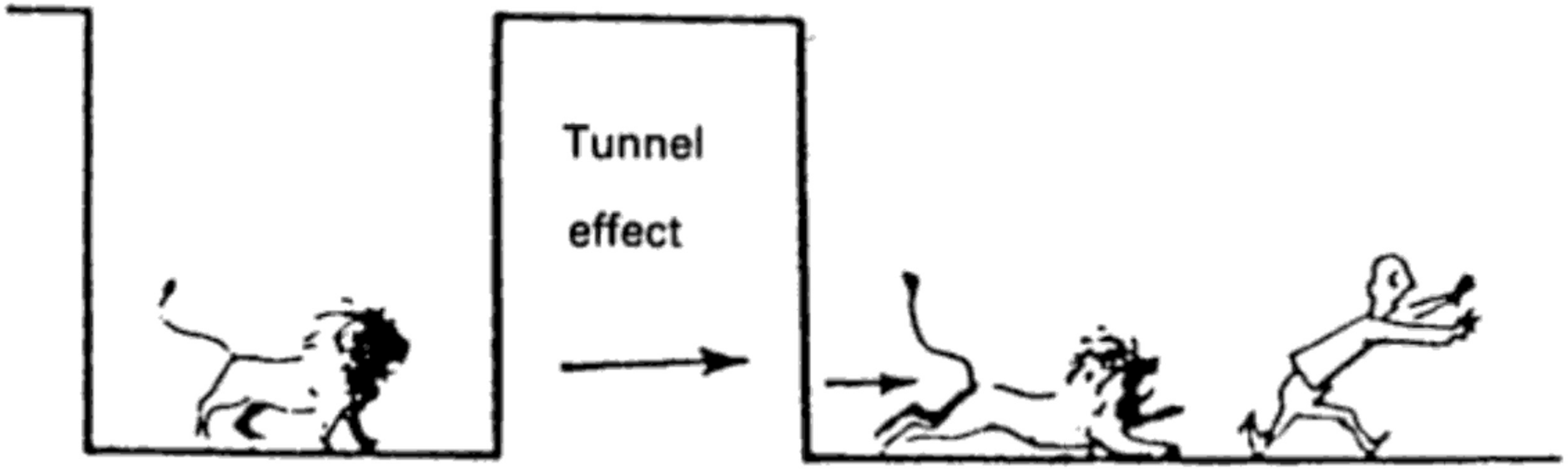




What does Quantum theory predict?



Credit: Bleaney '84



- Classical world

  Barrier region itself is forbidden, and this precludes particle motion on the far side as well.

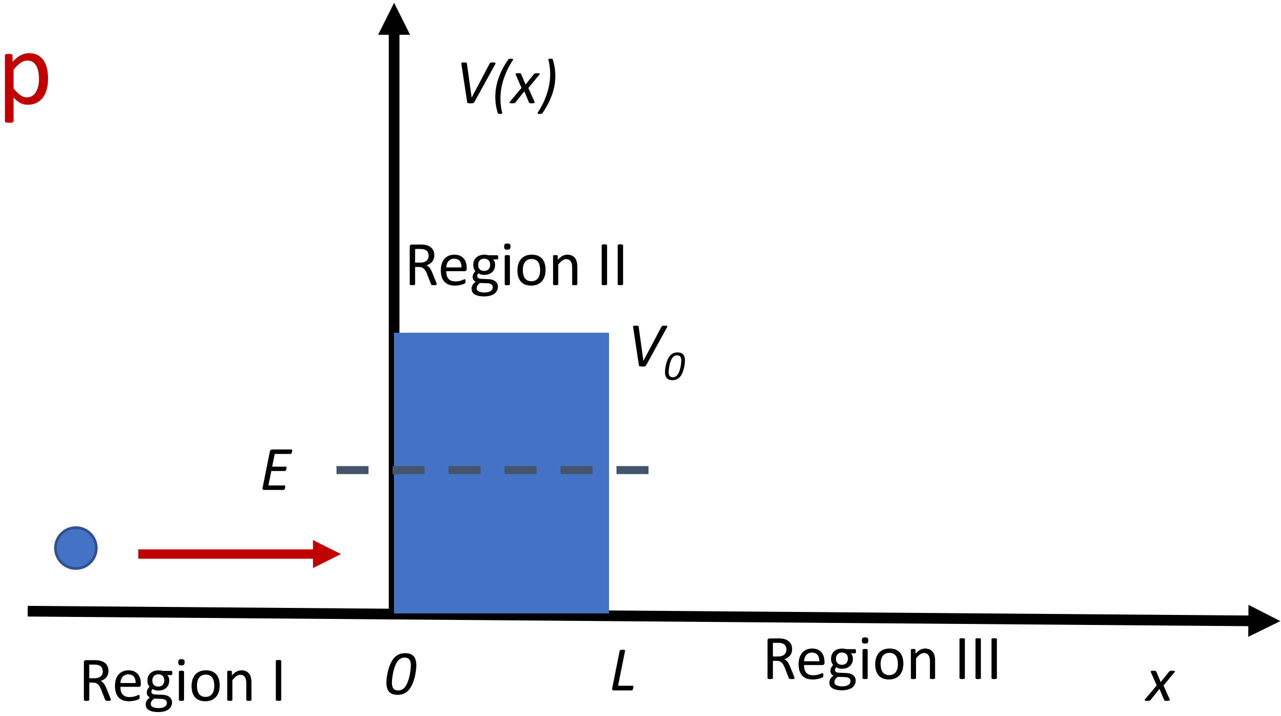
- Quantum World

  There is no inaccessible region to a particle. The matter wave associated with the particle is nonzero everywhere!

Finding the solutions

Finite Potential Barrier: Set up

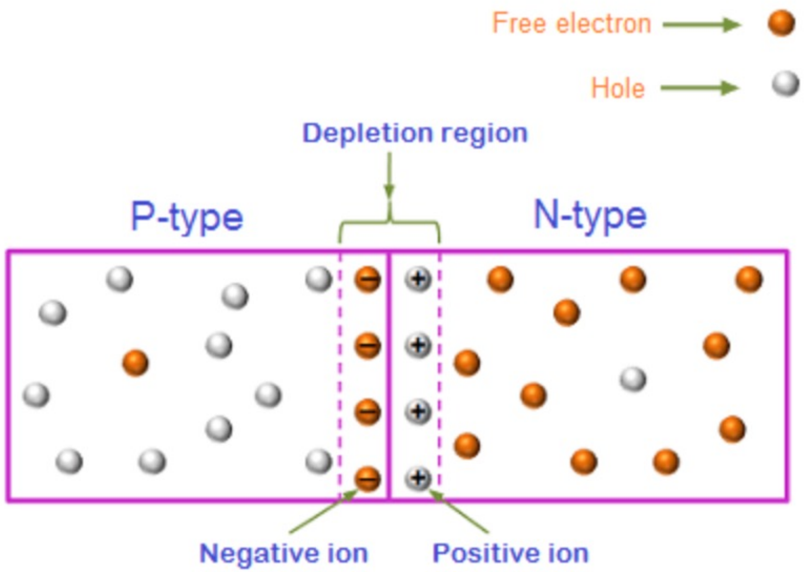
$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < L \\ 0 & x > L \end{cases}$$



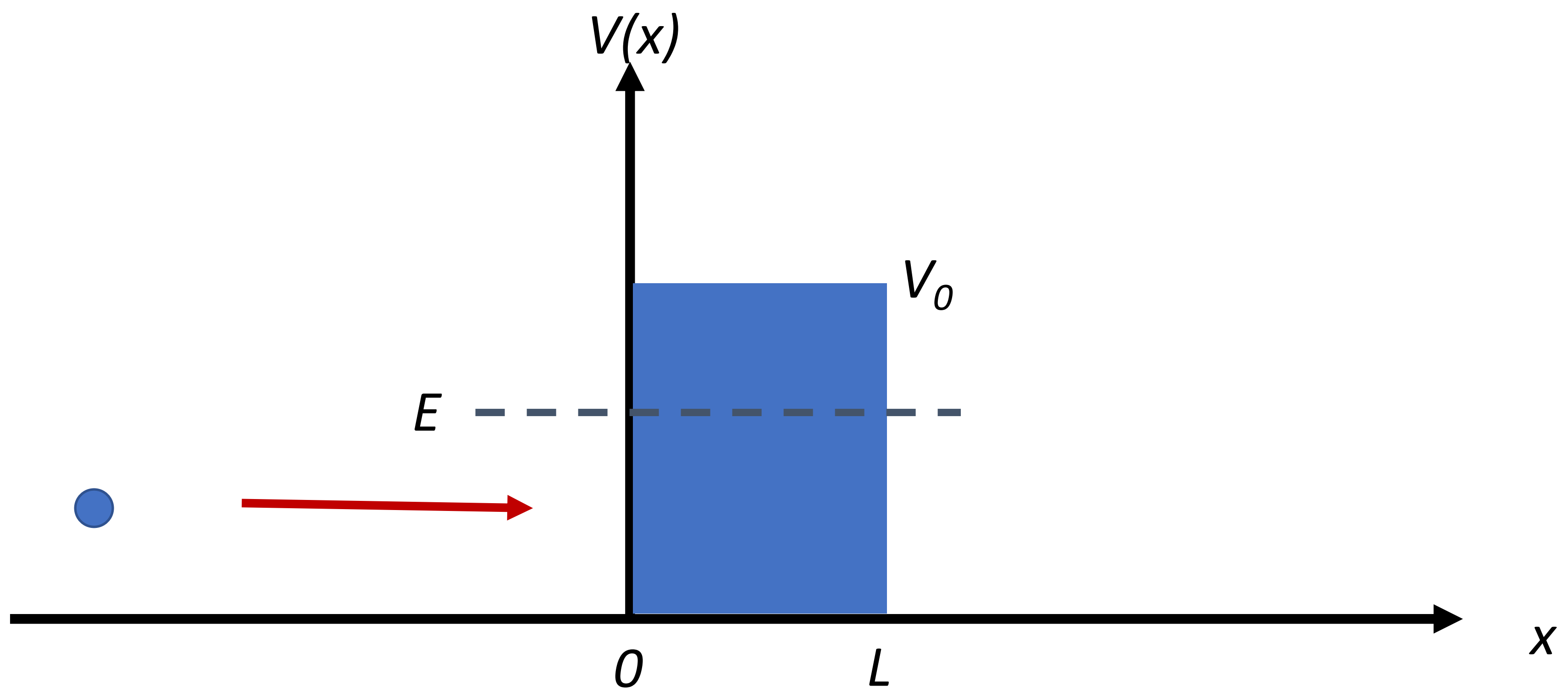
Physical system that can be approximated by a step potential:

1. Depletion region has different potential.

2. PE is constant inside P-Type and N-Type regions.



Finite Potential Barrier: Wave functions



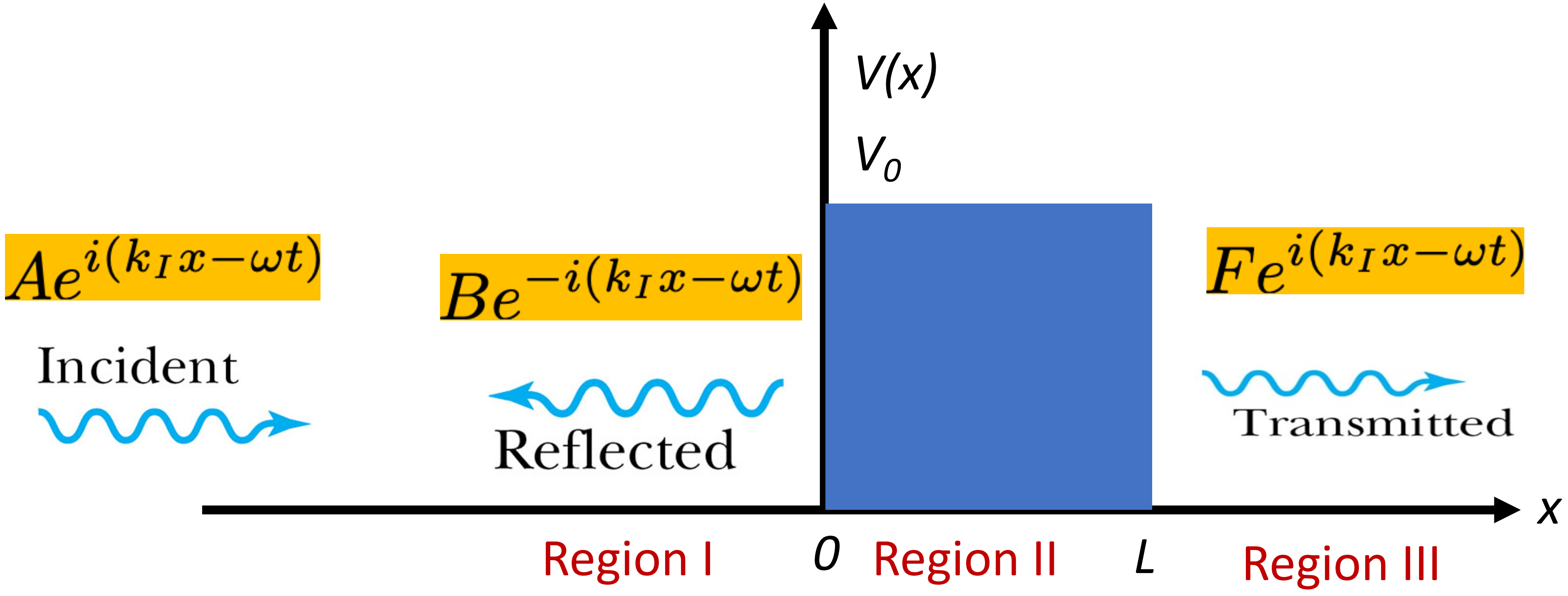
$x < 0$ and $x > L$

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

$0 < x < L$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E - V_0)\psi(x)$$

Finite Potential Barrier: Wave functions



$$x < 0 \text{ and } x > L \qquad\qquad 0 < x < L$$

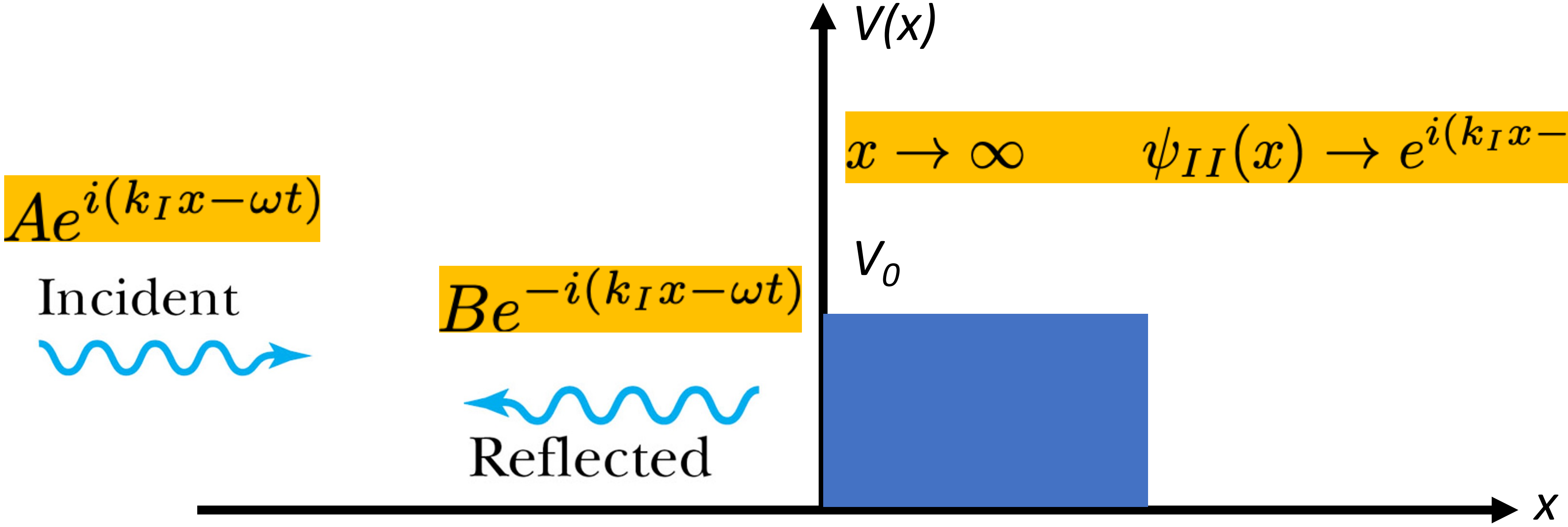
$$\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x} \qquad\qquad \psi_{II}(x) = Ce^{k_{II} x} + De^{-k_{II} x}$$

$$\psi_{III}(x) = Fe^{ik_I x} + Ge^{-ik_I x}$$

$$k_I = k_{III} = k = \sqrt{2mE}/\hbar \qquad\qquad k_{II} = \sqrt{2m(V_0 - E)}/\hbar$$

Finite Potential Barrier: Boundary condition 1

$$x \to \infty \qquad \psi_{II}(x) \to e^{i(k_I x - \omega t)} \implies G = 0$$



$x < 0$ and $x > L$

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_{III}(x) = Fe^{ikx}$$

$$k = \sqrt{2mE}/\hbar$$

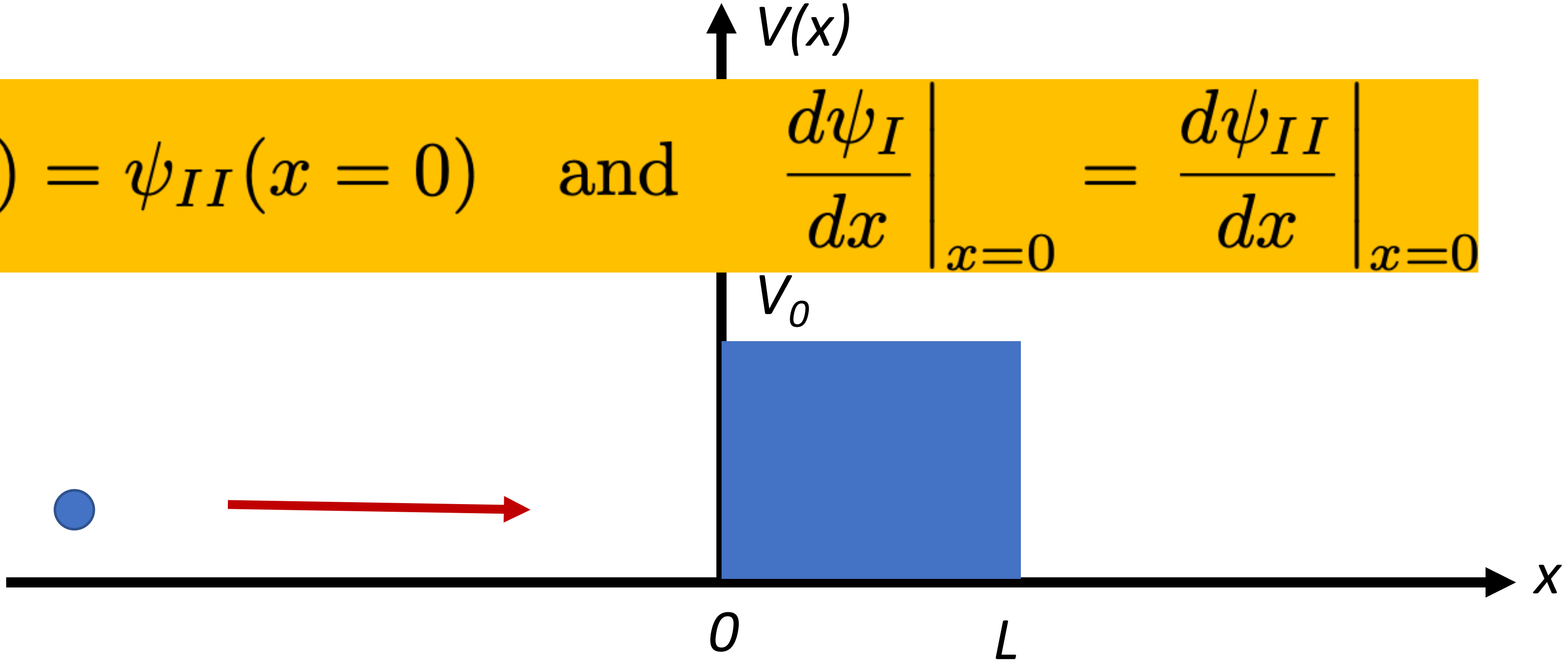
$0 < x < L$

$$\psi_{II}(x) = Ce^{k_{II}x} + De^{-k_{II}x}$$

$$k_{II} = \sqrt{2m(V_0 - E)}/\hbar$$

Finite Potential Barrier: Boundary conditions at x = 0

$$\psi_I(x=0) = \psi_{II}(x=0) \quad \text{and} \quad \left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0}$$



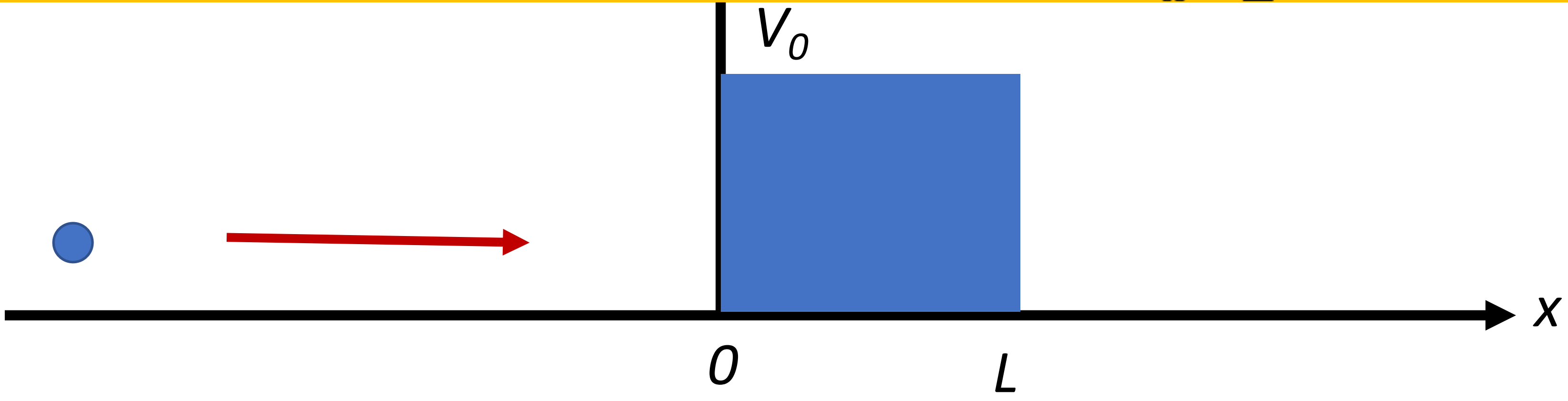
$$\left.Ce^{k_{II}x} + De^{-k_{II}x}\right|_{x=0} = \left.Ae^{ikx} + Be^{-ikx}\right|_{x=0} \implies C + D = A + B$$

$$k_{II}\left.(Ce^{k_{II}x} - De^{-k_{II}x})\right|_{x=0} = ik\left.(Ae^{ik_I x} - Be^{-ik_I x})\right|_{x=0} \implies \frac{ik_{II}}{k_I}(D - C) = A - B$$

A and B can be written in terms of C and D

Finite Potential Barrier: Boundary conditions at x = L

$$\psi_{II}(x=L) = \psi_{III}(x=L) \quad \text{and} \quad \left.\frac{d\psi_{II}}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}}{dx}\right|_{x=L}$$

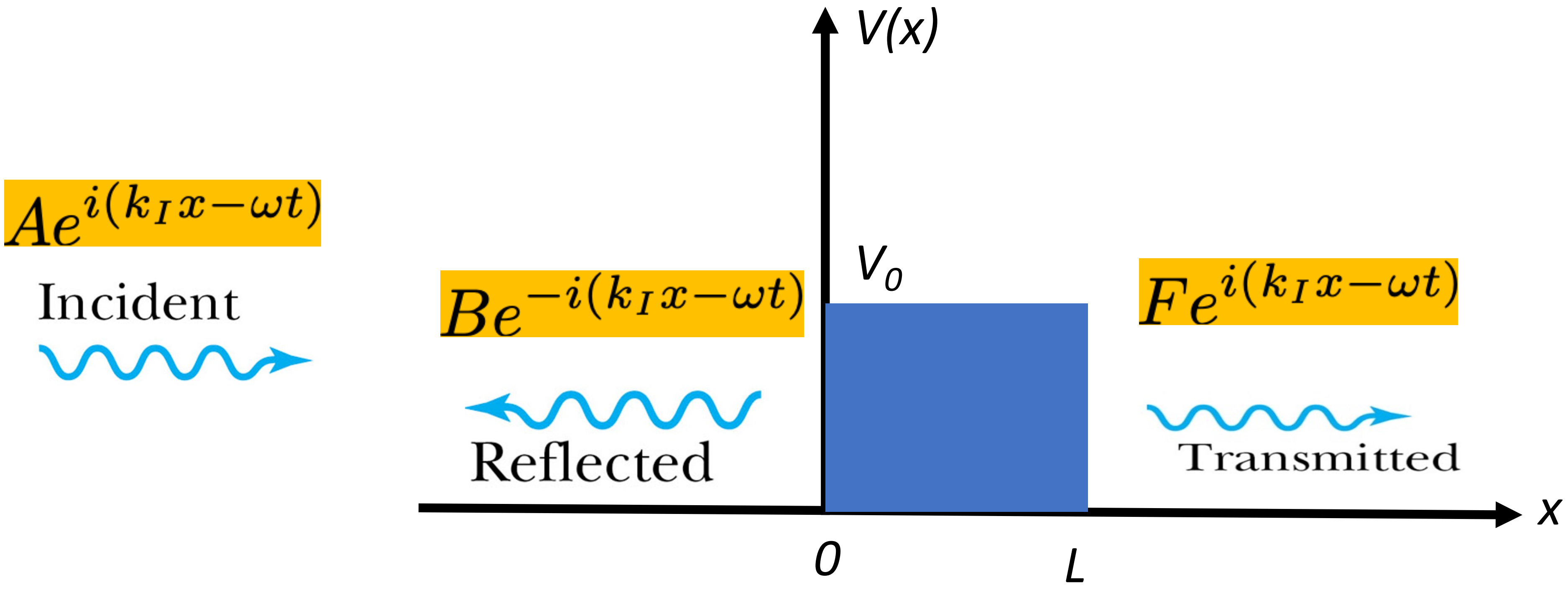


$$\left. Ce^{k_{II}x} + De^{-k_{II}x}\right|_{x=L} = \left. Fe^{ikx}\right|_{x=L} \implies Ce^{k_{II}L} + De^{-k_{II}L} = Fe^{ikL}$$

$$\left. k_{II}(Ce^{k_{II}x} - De^{-k_{II}x})\right|_{x=L} = \left. ikFe^{ikx}\right|_{x=L} \implies \frac{ik_{II}}{k}(De^{-k_{II}L} - Ce^{k_{II}L}) = Fe^{ikL}$$

C and D can be written in terms of F

Finite Potential Barrier: Final wave function

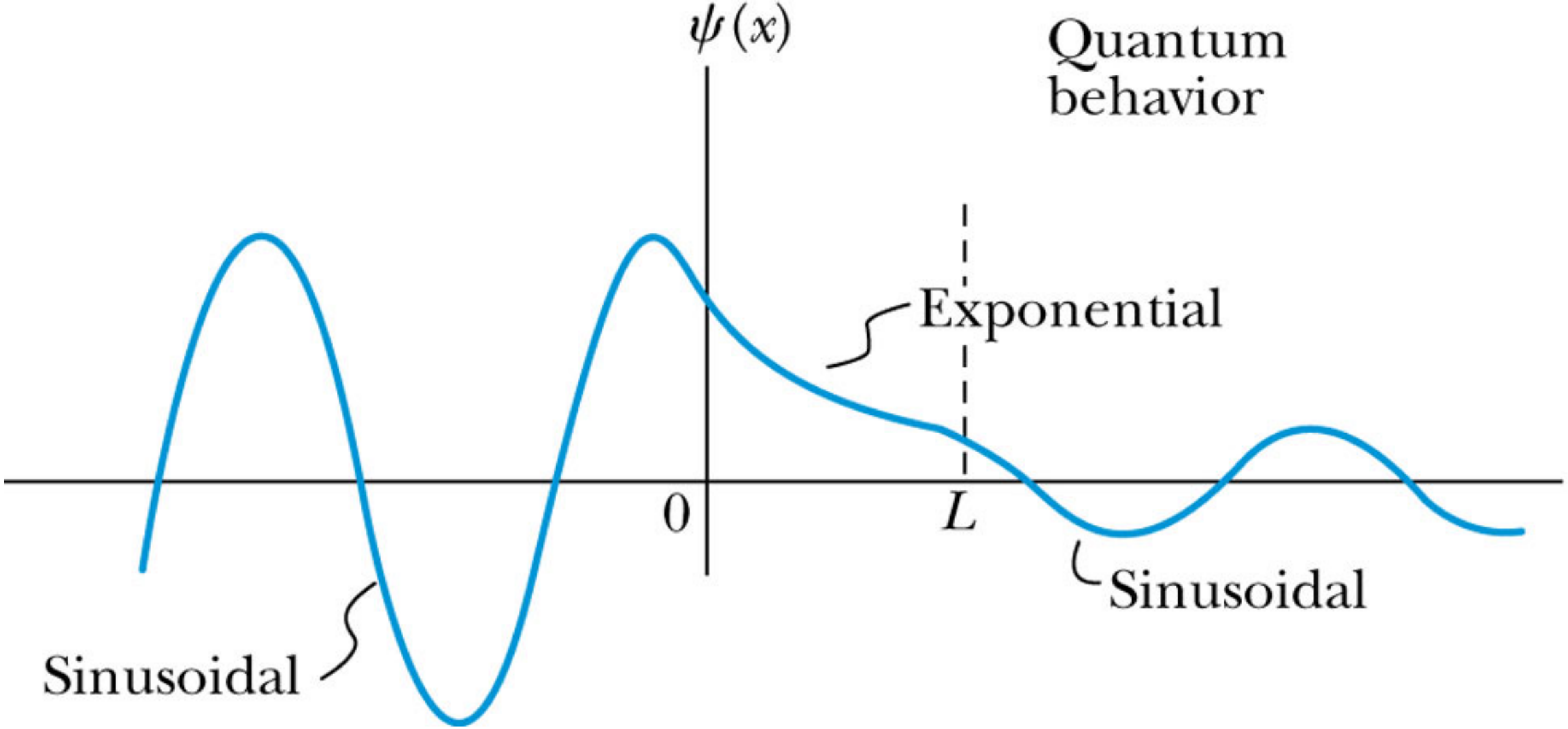


$$A = Fe^{ikL}\left[\cosh(k_{II}L) + \frac{k^2 - k_{II}^2}{2kk_{II}}\sinh(k_{II}L)\right] \qquad \psi_I(x) = Ae^{ikx} + Be^{-ik_I x}$$

$$B = -Fe^{ikL}\sinh(k_{II}L)\frac{k_{II}^2 + k^2}{2kk_{II}} \qquad \psi_{III}(x) = Fe^{ikx}$$

Wavefunction properties

Finite Potential Barrier: Visualizing wavefunction



Flux of particles: Definition

Classical context

- Consider *N* particles per unit length and each one has constant speed *v* in +ve *x*–direction.
- In Δ*t interval,* all particles within *u* Δ*t* will pass a fixed point.
- Particle flux (F) is number of particles passing a fixed point per unit time (like current):

$$F = \frac{Nv\Delta t}{\Delta t} = Nv$$

Quantum context

- Wavefunction corresponding to particles moving with definite momentum p is

$$\psi(x) = A\exp(ikx)$$

- We have $p = \hbar k \;\; and\; v = \frac{p}{m}$
- We know probability to find a free particle in same $\sim |A|^2$. Thus, average number of particles per unit length is $\sim |A|^2$.
- Flux of particles is $$F = |A|^2 \frac{\hbar k}{m}$$

Probability of Reflection and Transmission

- The probability of the particle being reflected (R) or transmitted (T) is:

$$\mathrm{R} = \frac{\text{flux of reflected particles}}{\text{flux of incident particles}}$$

$$\mathrm{T} = \frac{\text{flux of transmitted particles}}{\text{flux of incident particles}}$$

- Because the particle must be either reflected or transmitted:

$$R(E) = \frac{|\Psi_I(\text{Reflected})|^2}{|\Psi_I(\text{Incident})|^2} = \frac{|B|^2}{|A|^2}$$

$$T(E) = \frac{|\Psi_{III}(\text{Transmitted})|^2}{|\Psi_I(\text{Incident})|^2} = \frac{|F|^2}{|A|^2}$$

$$R(E) + T(E) = 1$$

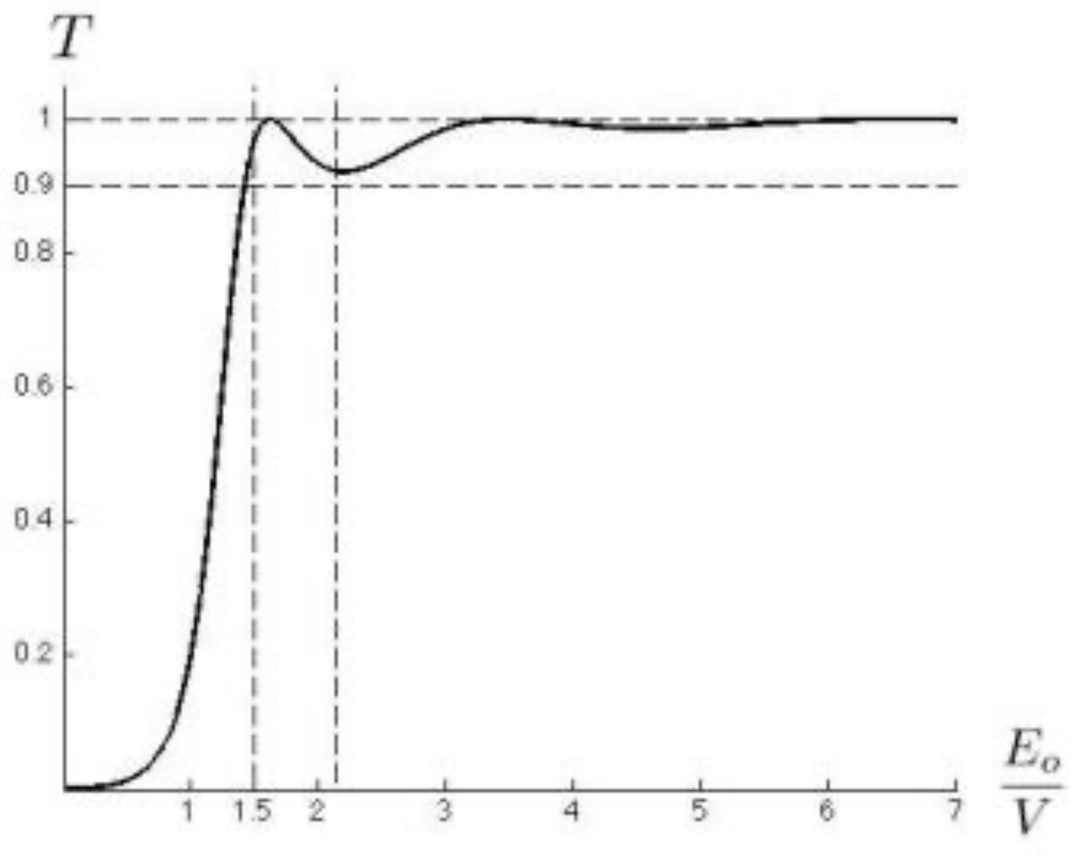
Probability of Reflection and Transmission

- Transmission probability is

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

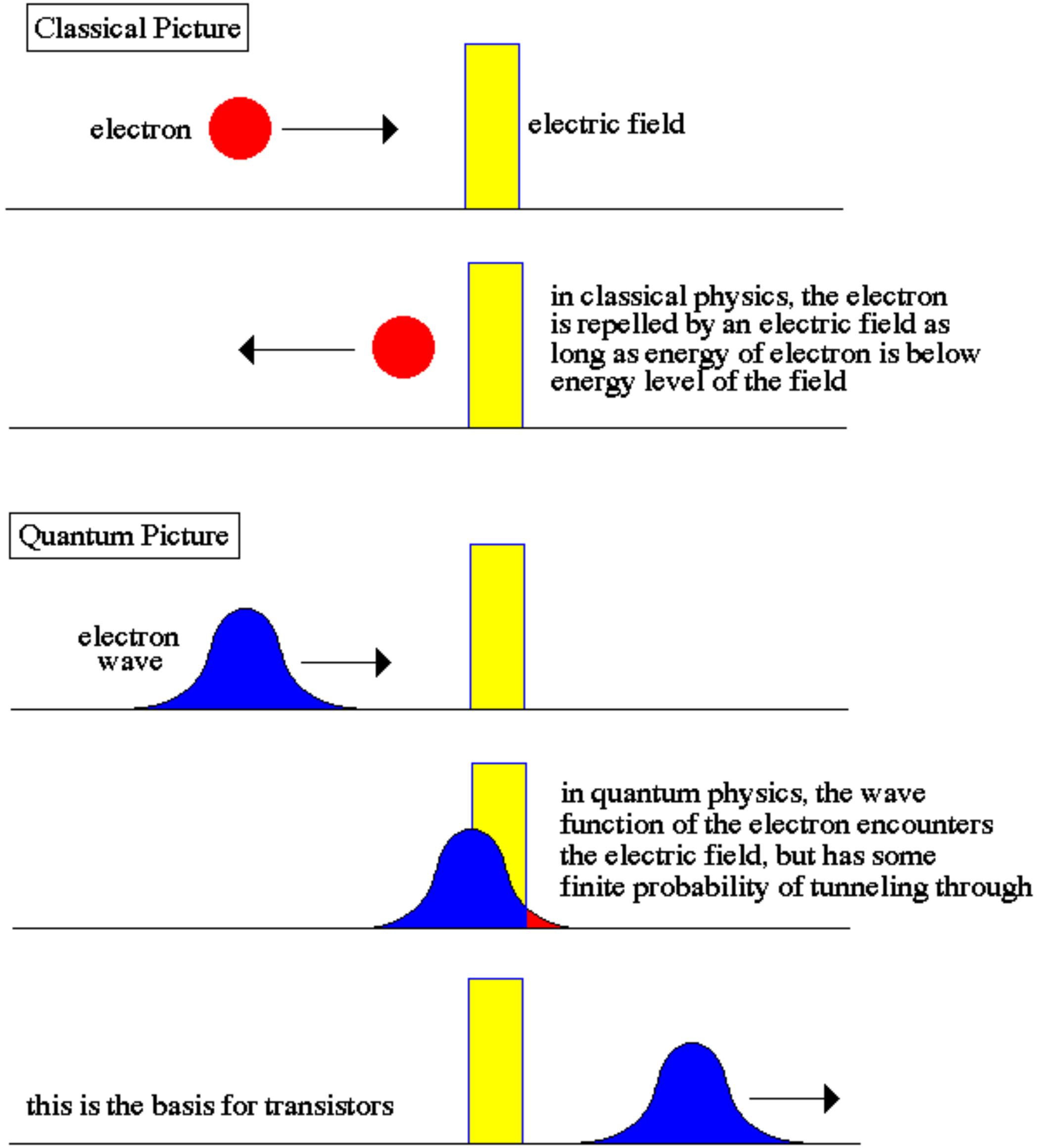
- The transmission probability describes the phenomenon of tunneling.

- Note that the transmission probability can be 1.



Transmission Coefficient versus E_o/V for barrier with $2m(2a)^2V/\hbar = 16$

Tunneling: Understanding



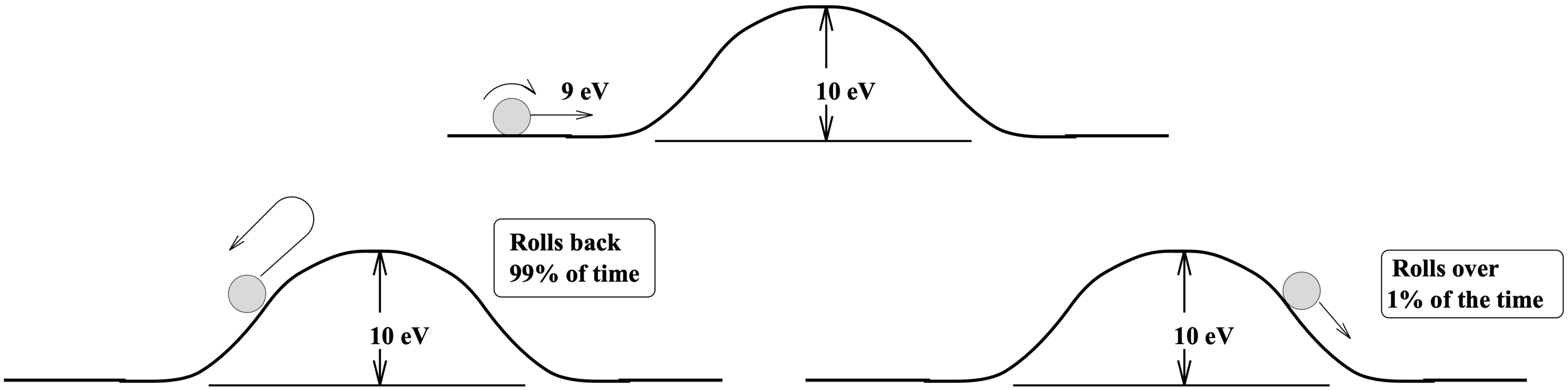
electron is always repelled

Why do we not see tunneling in our daily lives?

If the wall is much thicker than the quantum wavelength, Tunneling becomes improbable

- Electron usually repelled, but will occasionally pop out on the other side of the barrier.
- Probability of escape is small unless E is close to V_0.
- In that case, the particle may tunnel through the potential barrier and emerge with the same energy E.

Uncertainty Explanation



- $k_{II}L \gg 1$: Transmission probability becomes:

  Matches with the Step potential!

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

- The exponential shows the importance of the barrier width L over the barrier height V_0.

- 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:

$$\Delta E \simeq \frac{(\Delta p)^2}{2m} = V_0 - E$$

Uncertainty Explanation

- At the first sight the tunneling of a particle looks like a paradoxical problem, since if the height of the barrier is greater than the total energy of the particle, the kinetic energy is negative and *p* is imaginary.

- At the root of this paradox is our assumption that at each instant we know both the kinetic and the potential energy separately, or in other words we can assign values to the coordinate x and the momentum p simultaneously and this is in violation of the uncertainty principle.

- Question: Whether it is possible to determine the position of the particle when it is moving under the barrier or not?

- For this we observe that the particle can be at the point x where E<V(x) but then according to the uncertainty principle its momentum is uncertain by an amount $\sqrt{\overline{\Delta p^2}}$
- Thus if we know the position of the particle to be x, then its total energy cannot be E.

Uncertainty Explanation

- Since the transmission amplitude during tunneling is proportional to

$$\exp\left[-\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2m(V(x)-E)}dx\right]$$

  where x_0 is the point where E = 0.

- The probability of finding the particle which is coming from the left to be on the right of the barrier, i.e. $x_0 + b$ is proportional to the square of this amplitude or to the factor

$$\exp\left[-\frac{2}{\hbar}\int_{x_0}^{x_0+b}\sqrt{2m(V(x)-E)}dx\right]$$

- Now if we want a non-negligible probability then

$$2\sqrt{2m\left(V_m - E\right)}b \approx \hbar$$

  V_m is the maximum height of the potential.

- To find the position of the particle inside the barrier, we have to measure its coordinate with an accuracy $\Delta x < b$ therefore the uncertainty in momentum is

$$\overline{\Delta p^2} = \frac{\hbar^2}{4(\Delta x)^2} = \frac{\hbar^2}{4b^2}$$

- From the above two expressions, we have

$$\frac{\overline{\Delta p^2}}{2m} = V_m - E$$

Applications of Tunnelling

$$ {}^{A}_{Z}X \longrightarrow {}^{A-4}_{Z-2}Y + {}^{4}_{2}\alpha $$

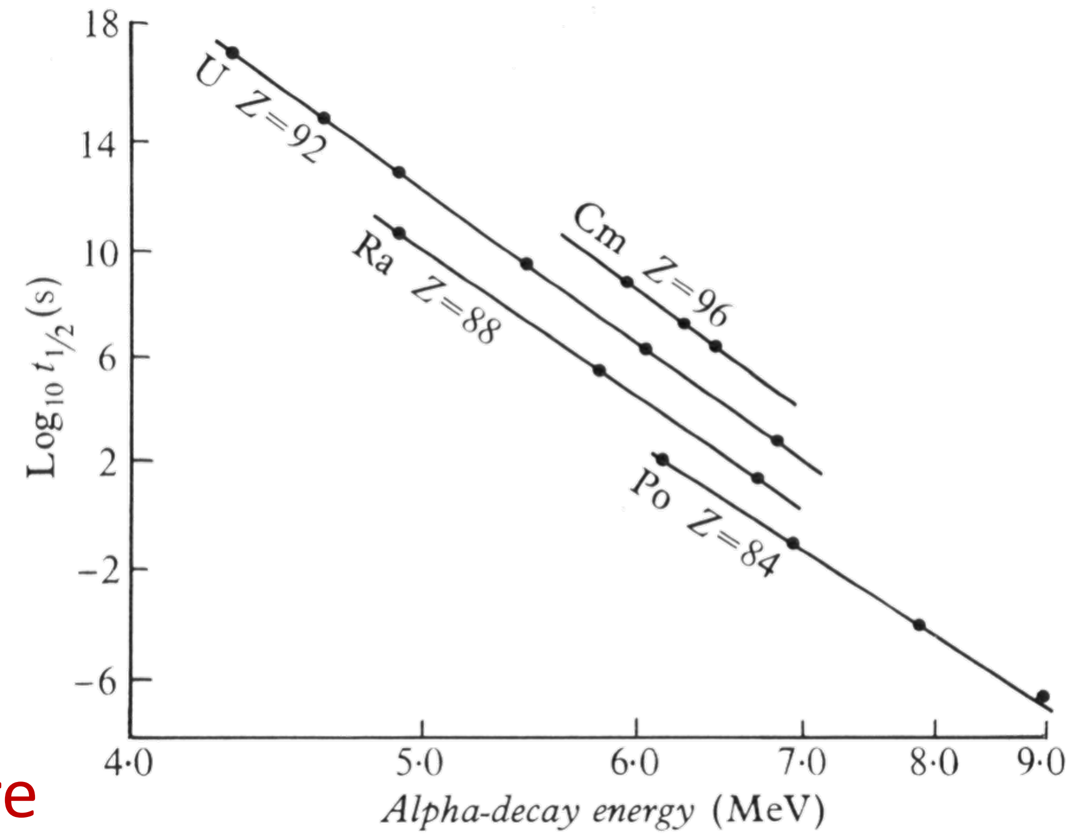
Alpha-Particle Decay: Gieger-Nuttal law

- Radioactive half lives vary from 10^{-6}s to 10^{17}s but the alpha decay energies only vary from 4 to 9 MeV

- Gieger-Nuttal law $$\log_{10} W = C - \frac{D}{\sqrt{T_\alpha}}$$

- *W* is the decay probability $\tau_{1/2} = \ln 2/W$
- T_α is KE of the alpha-particle

- Law states that Short-lived isotopes emit more energetic alpha particles than long-lived ones.



Experimental data of Geiger-Nuttall (1911)

Alpha-Particle Decay

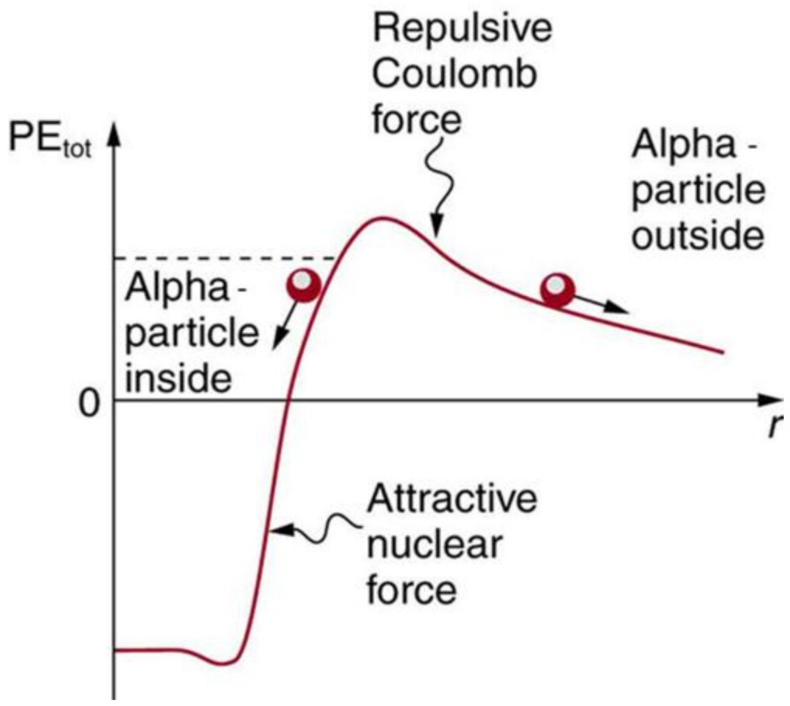
- Nuclei with A > 150 are unstable with respect to alpha decay A(Z,N) → A(Z-2,N-2) + α
- Nucleus spontaneously decays by emitting an alpha-particle (He particle).
- Effectively all the energy released goes into the kinetic energy of the α particle.

- Inside the nucleus, alpha particle feels strong, short-range attractive nuclear force as well as repulsive Coulomb force.
- Alpha-particles generally have only a few particles generally have only a few MeV of energy.

  How can they jump from the well?

- To escape from the nucleus, the alpha particle must tunnel through the barrier.

  This tunneling causes the observed radioactive decay.

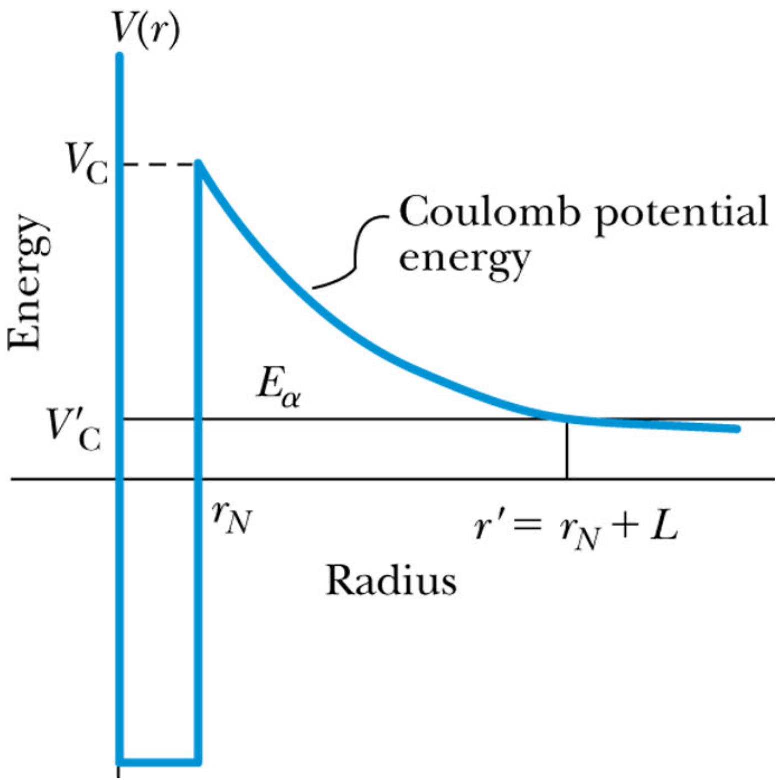


Alpha-Particle Decay

- Approximate the nuclear force dominates inside the nuclear radius as a square well.
- Height of the Coulomb barrier $V_C = \dfrac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r_n} = 37\,MeV$
- the tunneling distance L = 55 Fermi
- Assume $k_{II} L \gg 1$ $\quad T \sim e^{-2k_{II}L}$

$$k_{II} = \frac{\sqrt{2 \times 3727 MeV/c^2 \times (20 - 4.2) MeV}}{6.58 \times 10^{-22} MeV s} = 1.7 \times 10^{15}/\mathrm{m}$$

- $T \sim 2.4 \times 10^{-37}$



Alpha-Particle Decay: Theory and experiments

We can estimate the decay probability $W = P\,\nu\,T$

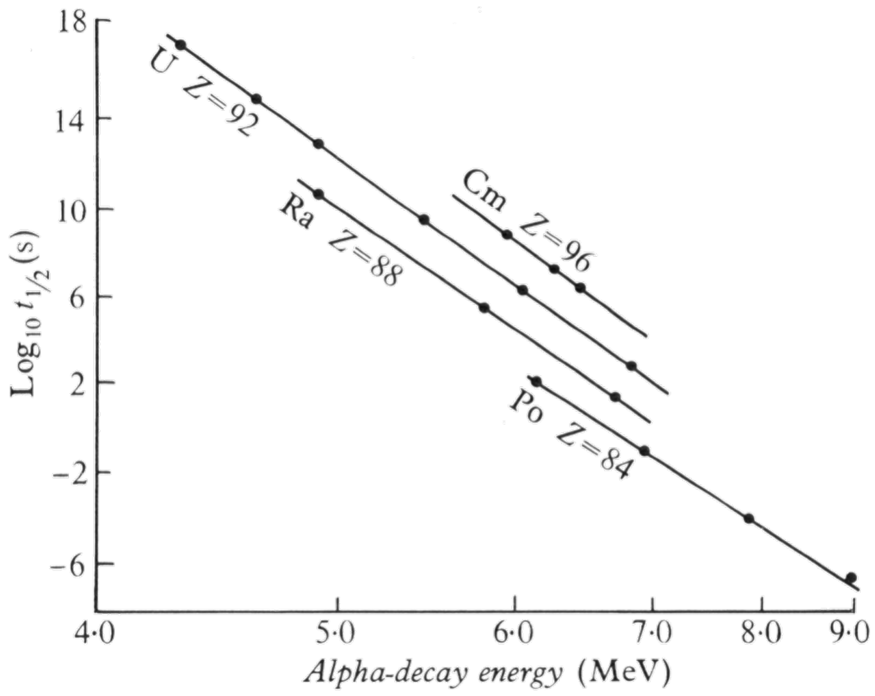
P is the probability of finding alpha in a nucleus (~ 0.1)

ν is the frequency that an alpha appears at the surface of the nucleus $\sim \frac{v}{R} \sim 10^{21}\ s^{-1}$

T is the transmission probability

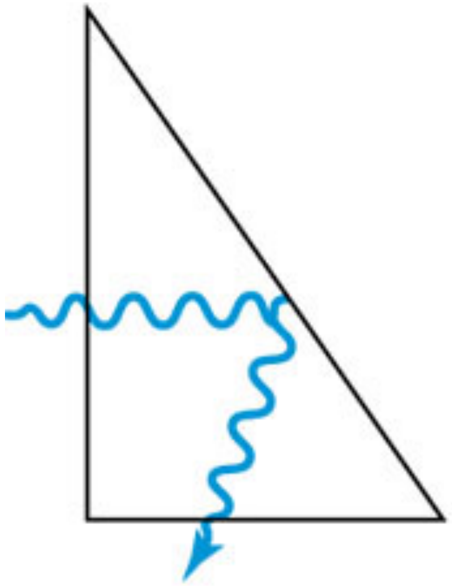
$$\tau_{1/2}(\text{theory}) = \frac{\ln 2}{W} = 2.8 \times 10^{16}\ \text{s}$$

$$\tau_{1/2}(\text{experiment}) = 1.4 \times 10^{17}\ \text{s}$$



Explanation for Frustrated total internal reflection

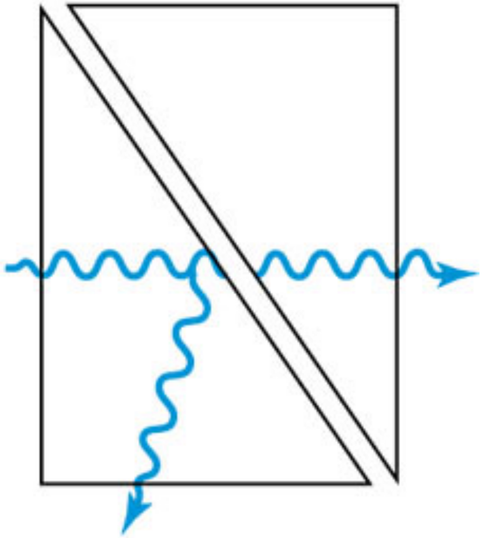
Experiment 1: Total Internal Reflection



- Consider a light passing through a glass prism.
- Light gets reflected from an internal surface with an angle greater than the critical angle.

Experiment 2: Frustrated total Internal Reflection

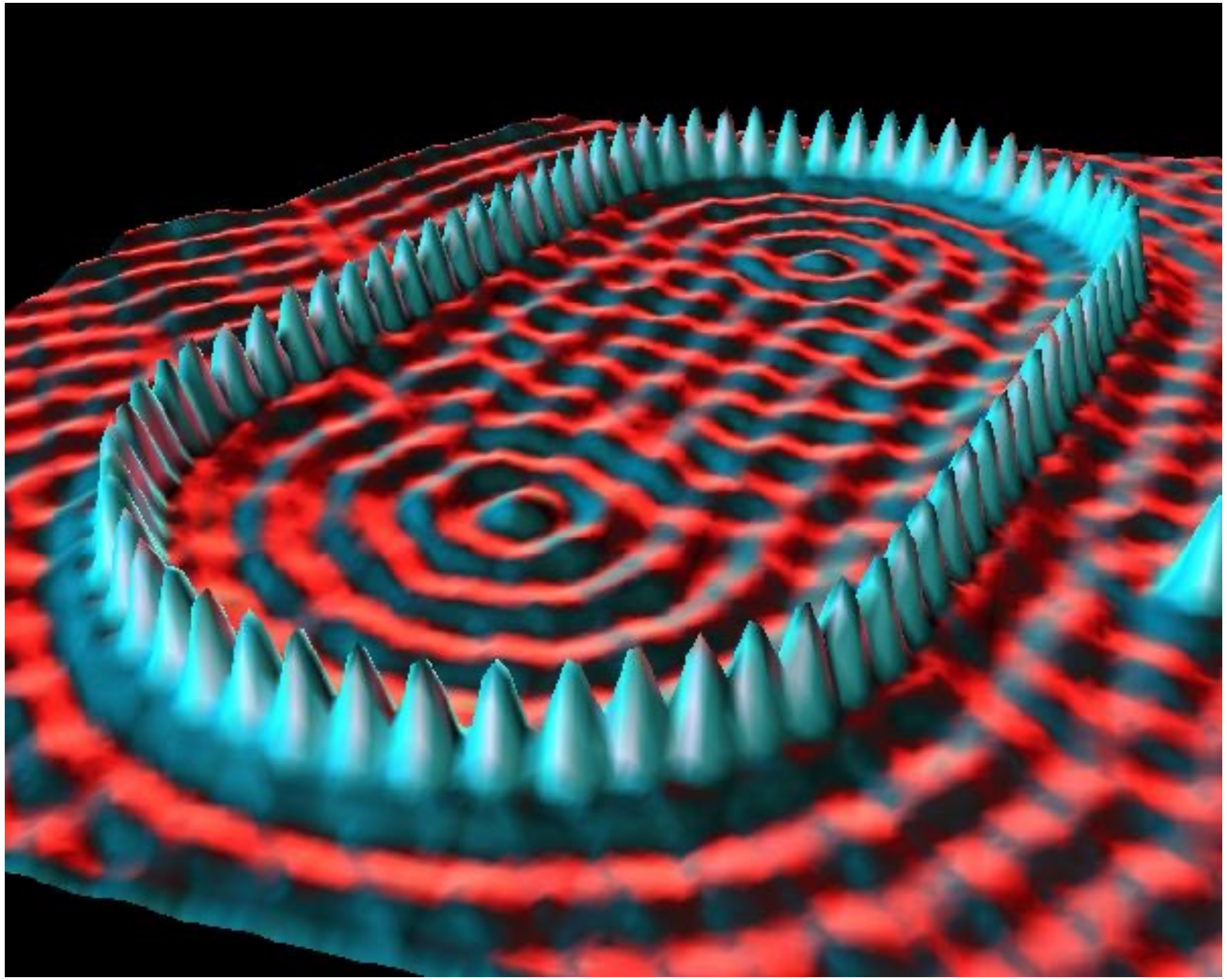
YouTube Video



- Let us bring another prism very close to the first one.
- Newton first observed that light appears in the second prism.
- The intensity of the second light beam decreases exponentially as the distance between the two prisms increases.

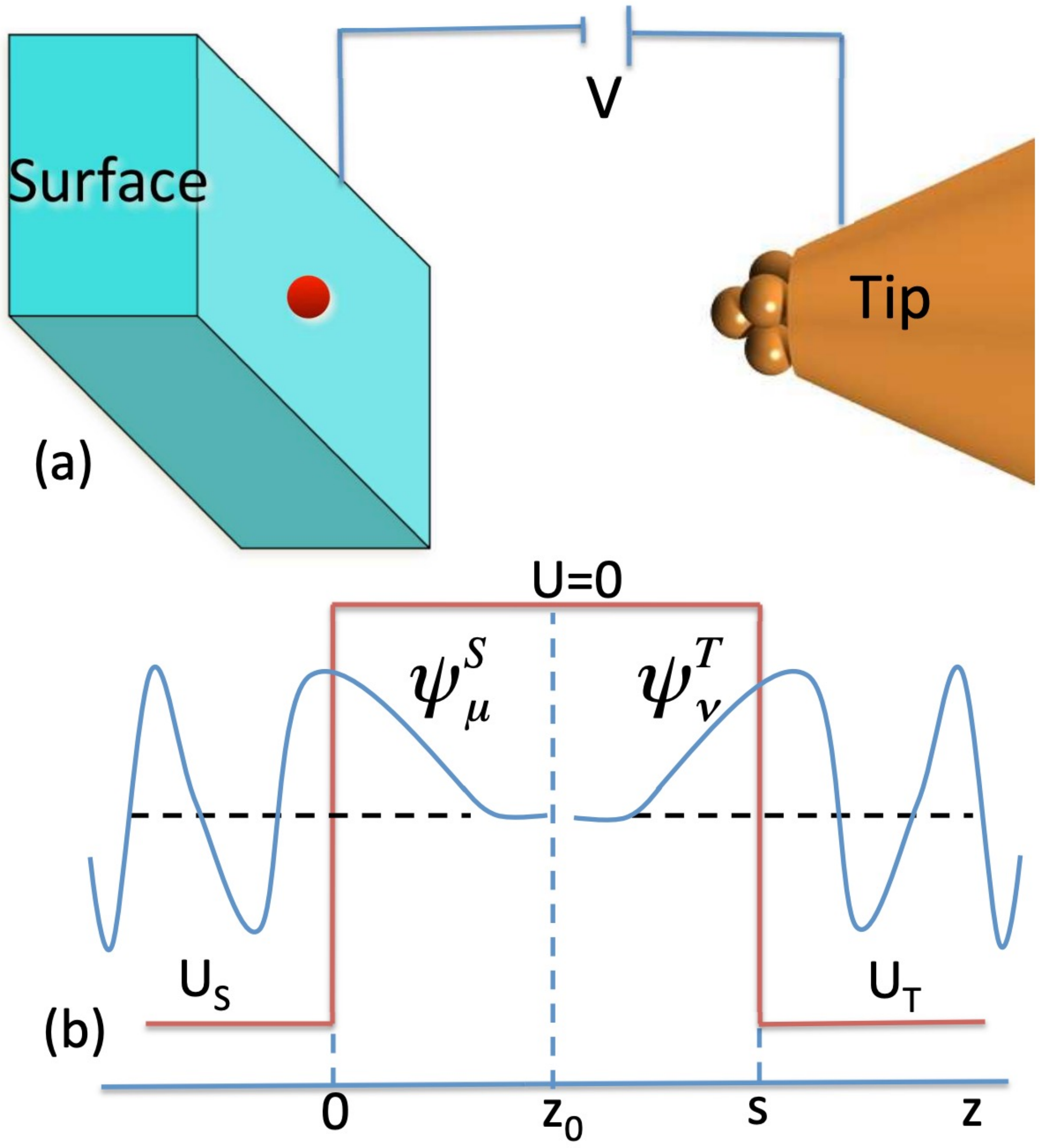
Light is not exactly zero just outside the prism.

Scanning Tunneling Microscope



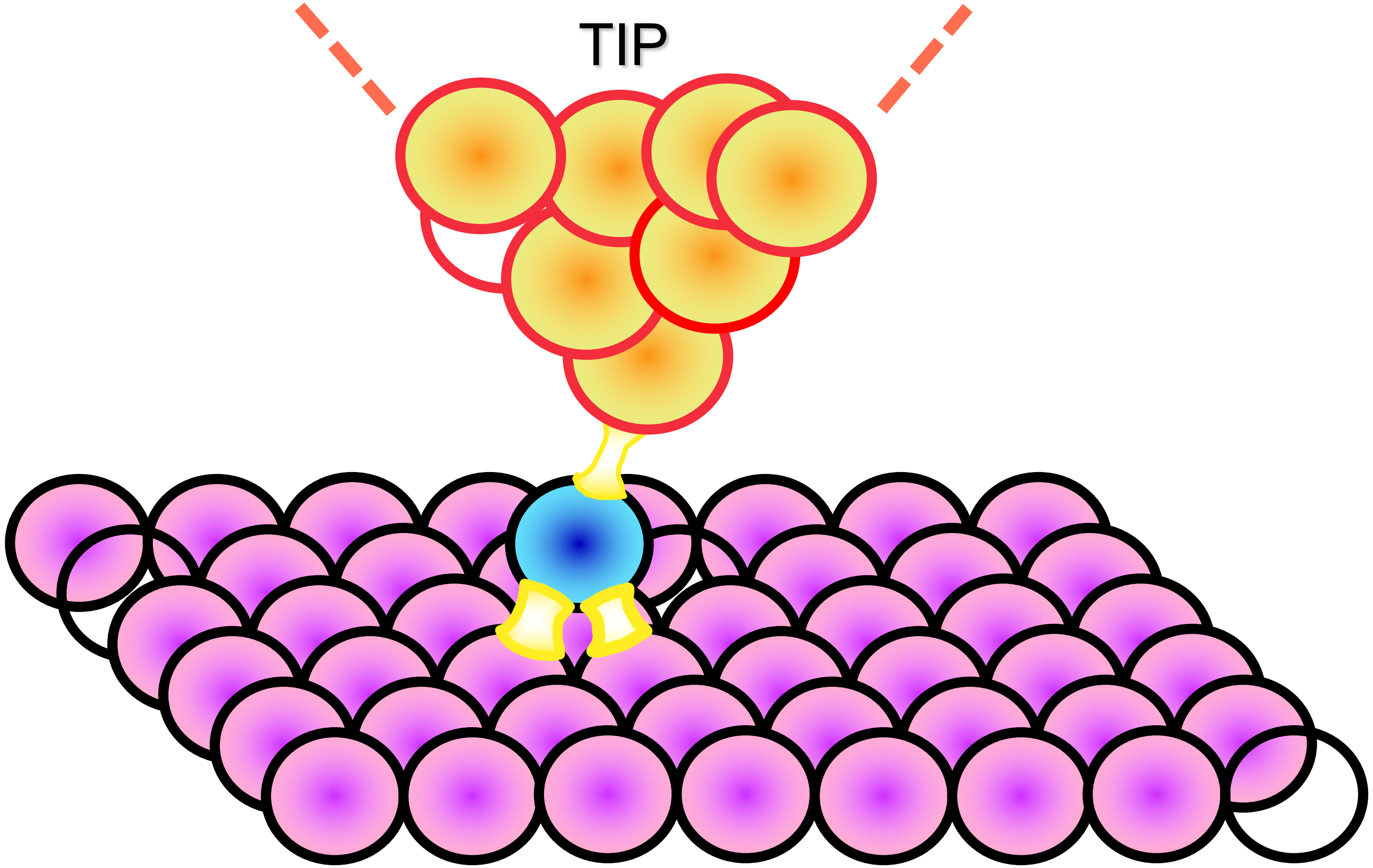
STM

- Invented by Gerd Binnig and Heinrich Rohrer in 1982
- Nobel prize in 1986!
- The basic idea makes use tunneling
  - When a sharp needle tip is placed less than 1 nm from a conducting material surface and a voltage applied between them, electrons can tunnel between the tip and surface
  - Since the tunnel current varies exponentially with the tip-surface distance, sub-nm changes in distance can be detected



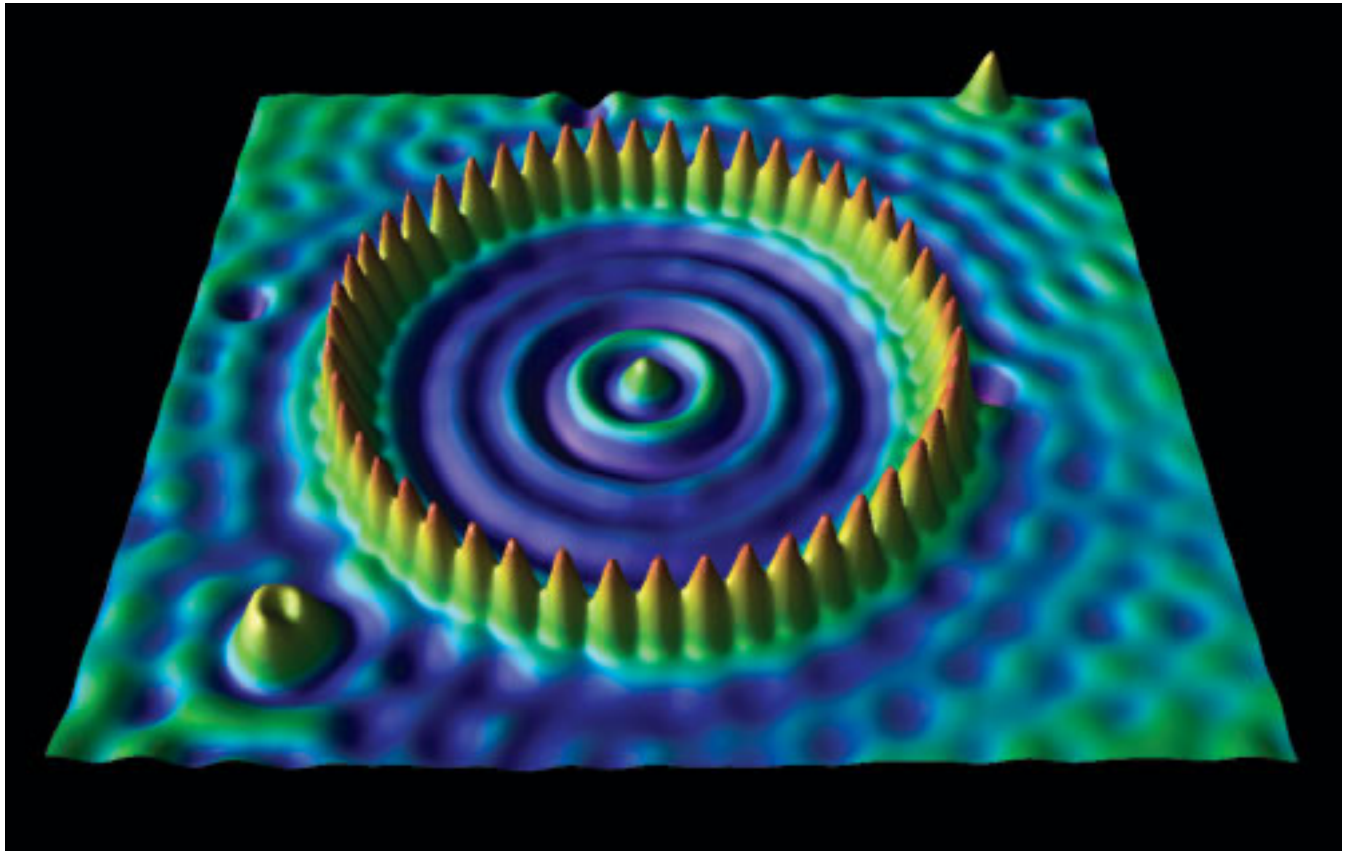
STM

- STM can also be used to manipulate atoms via van der Waals, tunneling, or electric field forces

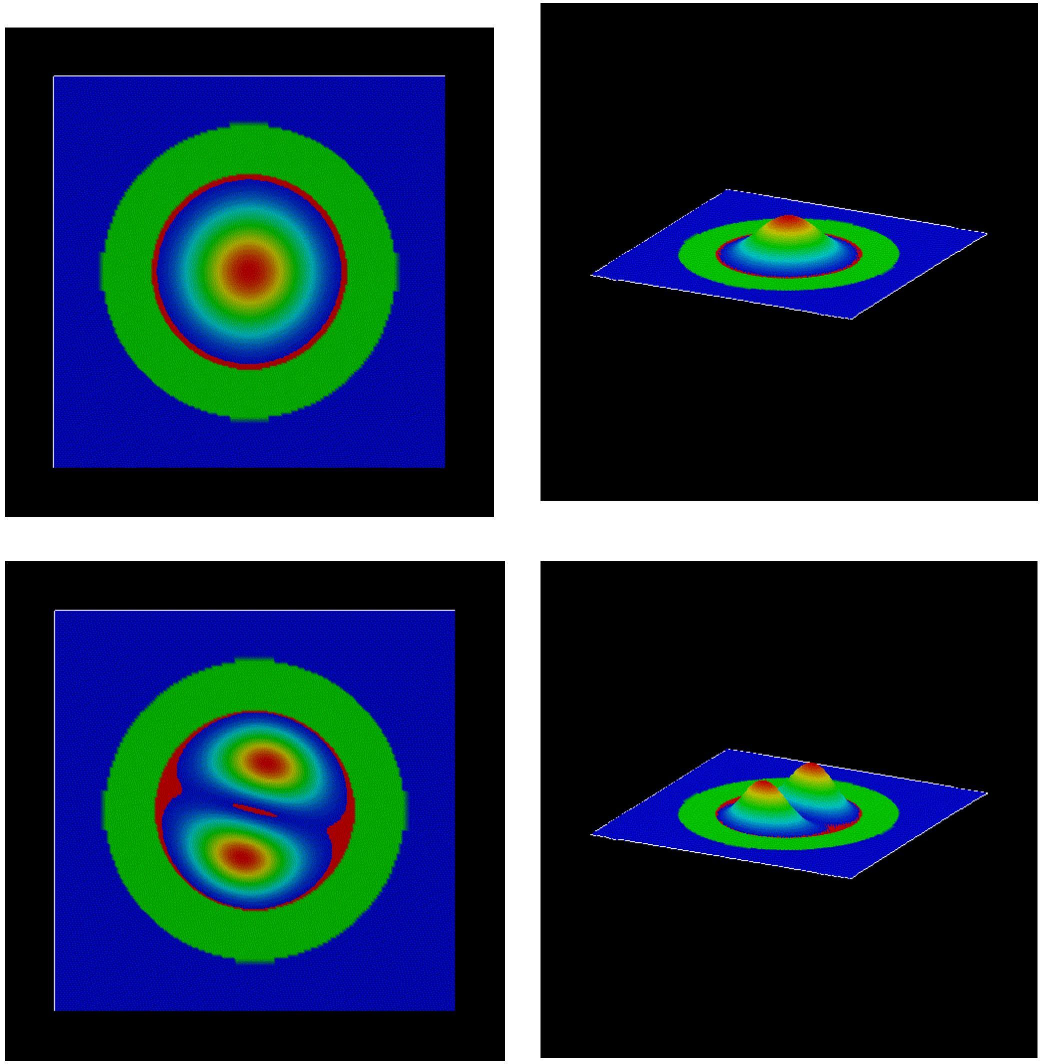


Quantum Corrals

Electron in a corral of iron atoms on copper



- Electron in a corral of iron atoms



Summary

- A quantum particle that is incident on an finite potential barrier and height may cross the barrier. It does not have a classical analog.

- Transmission coefficient is not zero.

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

- No classical analogue!

Recommended Reading

Tunnelling Chapter 7