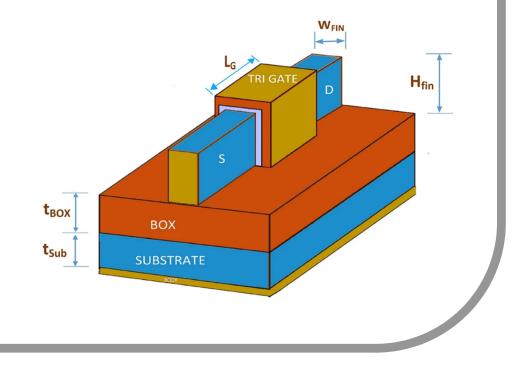
# Lecture 6

# **Schrödinger Equation: The Time-Independent Form**

#### In this lecture you will learn:

- Schrödinger equation the time-independent form
- Particle in an infinite potential well
- Quantum mechanical tunneling



Schrödinger Equation: What We Learned from the Previous Lecture

The mean value of the energy is:

$$\langle E \rangle (t) = \int_{-\infty}^{\infty} dx \, \psi^* (x,t) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t)$$

The total energy operator

The Schrodinger equation is:

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(\mathbf{x}) \right] \psi(\mathbf{x}, t)$$
  
The total energy operator



The potential is not explicitly time dependent

The total energy *E* of the particle, given by,

$$\boldsymbol{E} = \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 + \boldsymbol{V} \left( x \right)$$

**Energy Conservation in Newtonian Physics** 

is conserved, i.e.,

$$\frac{dE}{dt} = m\left(\frac{dx}{dt}\right)\left(\frac{d^2x}{dt^2}\right) + \frac{dV(x)}{dx}\left(\frac{dx}{dt}\right) = 0$$

Total energy is time-independent

**Using Newton's second law:** 

$$m\left(\frac{d^2x}{dt^2}\right) = -\frac{dV(x)}{dx}$$

V(x)

### Schrödinger Equation: Time-Independent Form (1D)

Many cases of practical interest involve problems in which the potential is not a function of time:

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(\mathbf{x},t)}{\partial \mathbf{x}^2} + V(\mathbf{x})\psi(\mathbf{x},t)$$

In these cases, the TOTAL energy of the particle DOES NOT CHANGE with time and therefore we seek solutions of the form:

$$\psi(\mathbf{x},t) = \phi(\mathbf{x}) e^{-t/\hbar t}$$

Normalization requirement gives:

$$\int_{-\infty}^{\infty} dx \,\psi^*(x,t) \psi(x,t) = \int_{-\infty}^{\infty} dx \,\phi^*(x) \phi(x) = 1$$

Schrödinger Equation: Time-Independent Form (1D)

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{x},t)}{\partial x^2} + V(\mathbf{x})\psi(\mathbf{x},t)$$

$$\psi(\mathbf{x},t) = \phi(\mathbf{x}) \mathbf{e}^{-i\frac{\mathbf{E}}{\hbar}t}$$
 Energy **E**

The mean value of the energy is:

$$\langle E \rangle(t) = \int_{-\infty}^{\infty} dx \,\psi^*(x,t) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t)$$

$$= \int_{-\infty}^{\infty} dx \,\psi^*(x,t) \left[ i\hbar \frac{\partial}{\partial t} \right] \psi(x,t)$$

$$= \int_{-\infty}^{\infty} dx \,\psi^*(x,t) \left[ i\hbar \frac{\partial \psi(x,t)}{\partial t} \right] = \int_{-\infty}^{\infty} dx \,\phi^*(x) e^{i\frac{E}{\hbar}t} \left[ E\phi(x) e^{-i\frac{E}{\hbar}t} \right]$$

$$= E \int_{-\infty}^{\infty} dx \, \phi^*(x) \phi(x) = E \longrightarrow \text{Independent of time}$$

The standard deviation in energy can be shown to be zero:

$$\left\langle \boldsymbol{E^2} \right
angle(t) - \left[ \left\langle \boldsymbol{E} \right
angle(t) 
ight]^2 = \mathbf{0}$$

So energy of the state is precise!

Schrödinger Equation: Time-Independent Form (1D)

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{x},t)}{\partial x^2} + V(\mathbf{x})\psi(\mathbf{x},t)$$
$$\psi(\mathbf{x},t) = \phi(\mathbf{x})e^{-i\frac{E}{\hbar}t}$$

Plug the solution form in the Schrödinger equation to get the <u>time-independent</u> form of the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}+V(x)\phi(x)=E\phi(x)$$

We need to solve this equation!

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\phi(x) = E\phi(x)$$
  
The total energy operator

### Schrödinger Equation: Time-Independent Form (3D)

Many cases of practical interest involve problems in which the potential is not a function of time:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$

In these cases, the TOTAL energy of the particle DOES NOT CHANGE with time and therefore we seek solutions of the form:  $\psi(\vec{r},t) = \phi(\vec{r})e^{-i\frac{E}{\hbar}t}$  Energy E

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\phi(\vec{r}) = E\phi(\vec{r})$$

We need to solve this equation! The solutions will represent states with fixed precise energies

# The Free Particle in 1D

### Consider a free particle in 1D

The potential energy V(x) is 0 everywhere:

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{x},t)}{\partial x^2} + V(\mathbf{x})\psi(\mathbf{x},t)$$
$$\psi(\mathbf{x},t) = \phi(\mathbf{x})e^{-i\frac{E}{\hbar}t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}=E\phi(x)$$

Assume:  $\phi(x) = Ae^{ikx}$  — Plane wave solution And:

$$-\frac{\hbar^{2}}{2m}\frac{\partial^{2}\phi(x)}{\partial x^{2}} = E\phi(x)$$

$$\Rightarrow \frac{\hbar^{2}k^{2}}{2m}Ae^{ikx} = EAe^{ikx}$$

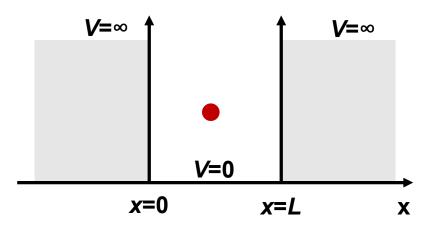
$$\Rightarrow E = \frac{\hbar^{2}k^{2}}{2m} \longrightarrow \psi(x,t) = Ae^{ikx}e^{-i\frac{E}{\hbar}t} = Ae^{ikx}e^{-i\frac{\hbar^{2}k^{2}}{2m}t}$$

0

Χ

### **Consider a particle placed inside a 1D box**

Inside the box the potential energy V(x) is 0 Outside the box the potential energy V(x) is  $\infty$ 

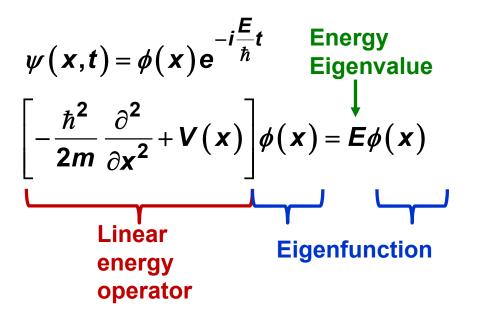


The infinite potential at the boundary walls (at x=0 and at x=L) ensure that the particle has no chance of ever being outside the box

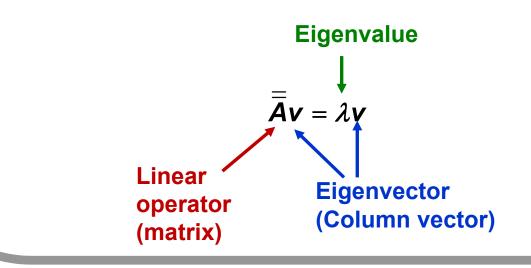
We need to figure out the quantum mechanical behavior of the confined particle:

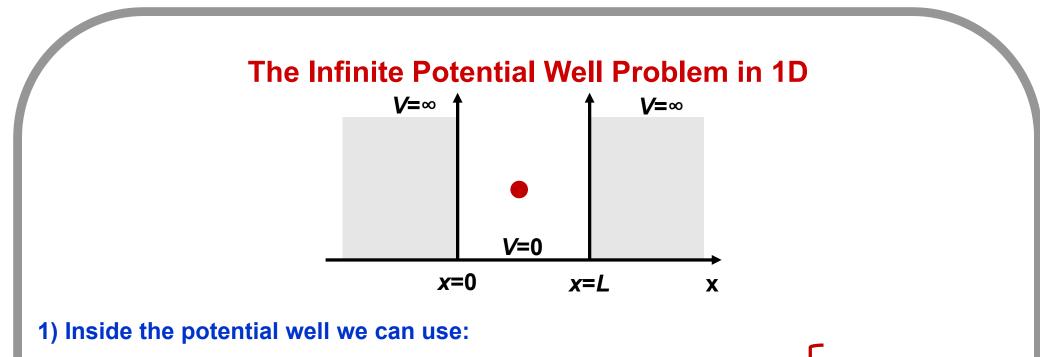
$$\psi(\mathbf{x},t) = \phi(\mathbf{x}) e^{-i\frac{E}{\hbar}t}$$
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi(\mathbf{x})}{\partial x^2} + V(\mathbf{x})\phi(\mathbf{x}) = E\phi(\mathbf{x})$$

### The Time-Independent Schrodinger Equation: An Eigenvalue Equation



Compared with a matrix eigenvalue equation:





$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} = E\phi(x) \qquad - V(x)=0 \text{ inside}$$

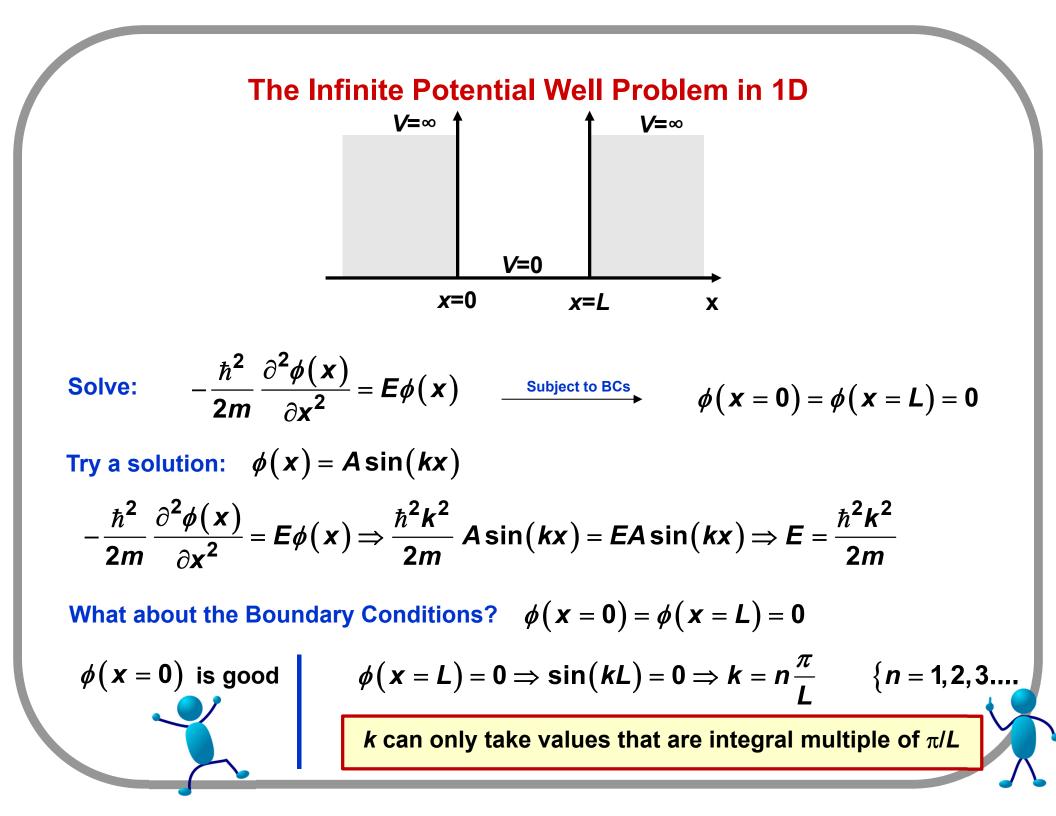
2) Outside the potential well we must have:  $\phi(x) = 0$ 

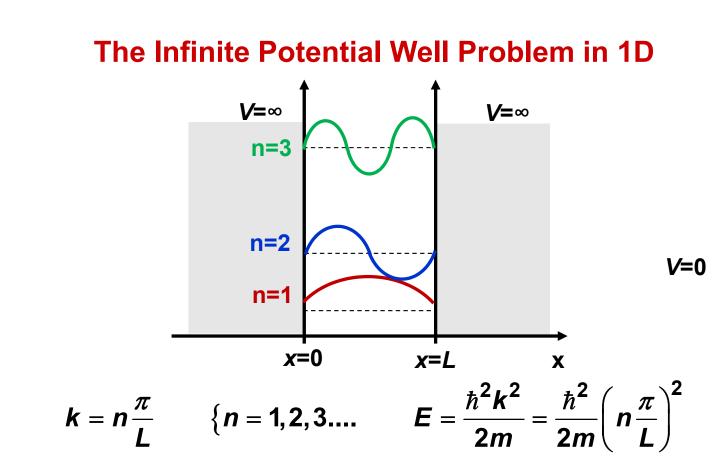
Otherwise the average potential energy of the particle will be infinite:  $- \left\{ V(x) \right\} = \int_{-\infty}^{\infty} dx \ \phi^*(x) \left[ V(x) \right] \phi(x)$ 

This is a second order differential equation  $\rightarrow$  needs two boundary conditions!

$$\phi(\mathbf{x}=\mathbf{0})=\phi(\mathbf{x}=\mathbf{L})=\mathbf{0}$$

So that the energy of the particle must not become infinite!





So the corresponding solutions are:

$$\phi_n(\mathbf{x}) = \mathbf{A}\sin\left(n\frac{\pi}{L}\mathbf{x}\right)$$
 { $n = 1, 2, 3....$ 

And the corresponding energies are:  $E_n = \frac{\hbar^2}{2m} \left( n \frac{\pi}{L} \right)^2$ 

**Energy quantization!** 

### **Proper normalization:**

We must have:

$$\int_{-\infty}^{\infty} dx |\phi_n(x)|^2 = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} dx |A|^2 \sin^2 \left(n \frac{\pi}{L} x\right) = 1$$

$$\Rightarrow |A|^2 = \frac{2}{L}$$

$$\Rightarrow |A| = \sqrt{\frac{2}{L}} e^{i\phi}$$

Choose the phase  $\phi$  to be 0:

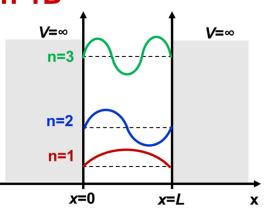
$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\frac{\pi}{L}x\right)$$

♦

$$\boldsymbol{E}_{\boldsymbol{n}} = \frac{\hbar^2}{2m} \left( \boldsymbol{n} \frac{\pi}{L} \right)^2$$

{*n* = 1, 2, 3....

$$\phi_n(x) = A \sin\left(n\frac{\pi}{L}x\right)$$
$$E_n = \frac{\hbar^2}{2m}\left(n\frac{\pi}{L}\right)^2$$



#### **Orthogonality of the solutions:**

**Different solutions are orthogonal** 

$$\int_{-\infty}^{\infty} dx \, \phi_m^*(x) \phi_n(x) = \delta_{nm}$$

As you will see, this is a very general property of the solutions of the time-independent Schrödinger equation

**V**=∞

n=3

**n=2** 

n=1

x=0

**∨**=∞

х

x=L

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\frac{\pi}{L}x\right)$$

$$\{n = 1, 2, 3....$$

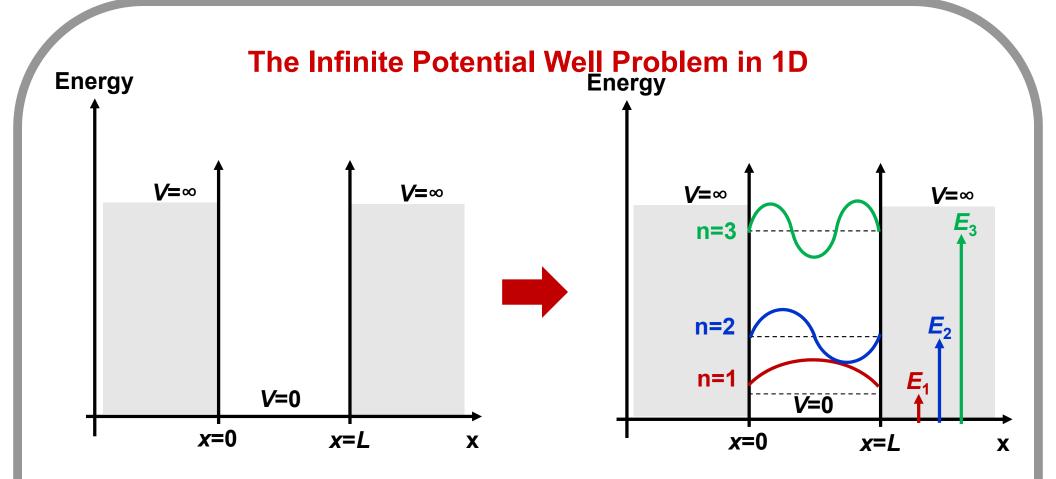
$$E_n = \frac{\hbar^2}{2m} \left(n\frac{\pi}{L}\right)^2$$



$$\psi(\mathbf{x},t) = \phi(\mathbf{x}) e^{-i\frac{E}{\hbar}t}$$

Solutions of the time-dependent Schrödinger equation for the infinite well would look like:

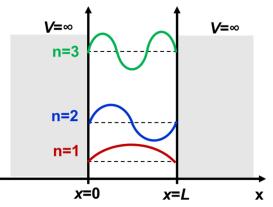
If: 
$$\psi(\mathbf{x}, t = \mathbf{0}) = \phi_n(\mathbf{x})$$
  $\{n = 1, 2, 3, ..., \\ \Rightarrow \psi(\mathbf{x}, t) = \phi_n(\mathbf{x}) e^{-i\frac{E_n}{\hbar}t}$   $\{n = 1, 2, 3, ..., \\ i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\mathbf{x}, t)}{\partial x^2} + V(x)\psi(x, t)$ 



### **Superposition in Quantum Mechanics**

Schrödinger equation is a linear differential equation

This means that a <u>superposition</u> (i.e a sum) of functions that satisfy the equation will also satisfy the equation



For the infinite potential well, since we have found that the following functions satisfy the Schrodinger equation:

$$\phi_n(\mathbf{x}) \mathbf{e}^{-i \frac{\mathbf{E}_n}{\hbar} t} \{ n = 1, 2, 3.... \}$$

Therefore, a superposition (i.e. a sum) of these functions, weighted by arbitrary complex coefficients, will also satisfy the time-dependent Schrodinger equation:

$$\psi(\mathbf{x},t) = \sum_{n} a_{n} \phi_{n}(\mathbf{x}) e^{-i\frac{E_{n}}{\hbar}}$$

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(\mathbf{x},t)}{\partial x^2} + V(\mathbf{x})\psi(\mathbf{x},t)$$

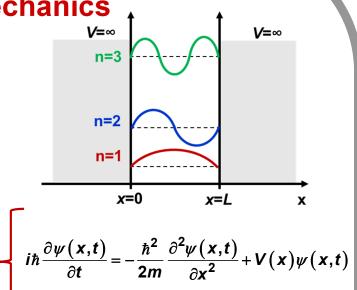
Complex coefficients

### **Superposition in Quantum Mechanics**

$$\psi(\mathbf{x},t) = \sum_{n} a_{n} \phi_{n}(\mathbf{x}) e^{-i\frac{E_{n}}{\hbar}t}$$

#### **Complex coefficients**

This solution does not have a fixed precise energy.
It is a <u>superposition</u> of states each of which has a fixed precise energy.



#### **Normalization:**

$$\int_{-\infty}^{\infty} dx \, \psi^*(x,t) \psi(x,t) = 1$$

$$\Rightarrow \sum_{n} \sum_{m} a_n^* a_m \int_{-\infty}^{\infty} dx \, \phi_n^*(x) e^{i\frac{E_n}{\hbar}t} \left[ \phi_m(x) e^{-i\frac{E_m}{\hbar}t} \right] = \sum_{n} \sum_{m} a_n^* a_m e^{i\frac{E_n}{\hbar}t} e^{-i\frac{E_m}{\hbar}t} \delta_{nm} = 1$$

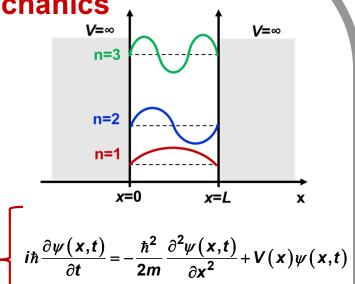
$$\Rightarrow \sum_{n} |a_n|^2 = 1$$

### **Superposition in Quantum Mechanics**

$$\psi(\mathbf{x},t) = \sum_{n} a_{n} \phi_{n}(\mathbf{x}) e^{-i\frac{E_{n}}{\hbar}t}$$

#### **Complex coefficients**

This solution does not have a fixed precise energy.
It is a <u>superposition</u> of states each of which has a fixed precise energy.

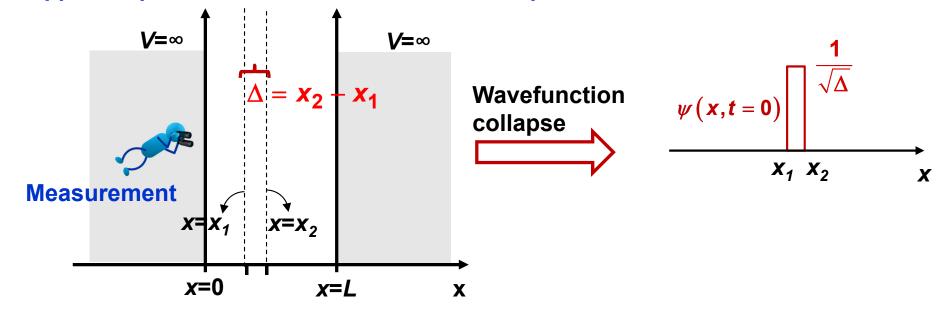


#### Mean energy:

$$\langle E \rangle(t) = \int_{-\infty}^{\infty} dx \, \psi^*(x,t) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t)$$
  
= 
$$\int_{-\infty}^{\infty} dx \, \psi^*(x,t) \left[ i\hbar \frac{\partial}{\partial t} \right] \psi(x,t) = \sum_{m} \sum_{n} a_n^* a_m \int_{-\infty}^{\infty} dx \, \phi_n^*(x) e^{i\frac{E_n}{\hbar}t} \left[ E_m \phi_m(x) e^{-i\frac{E_m}{\hbar}t} \right]$$
  
= 
$$\sum_{n} |a_n|^2 E_n$$

# The Infinite Potential Well Problem in 1D: A Post Measurement Time Evolution Problem

Suppose a particle is known to be in a infinite potential well box

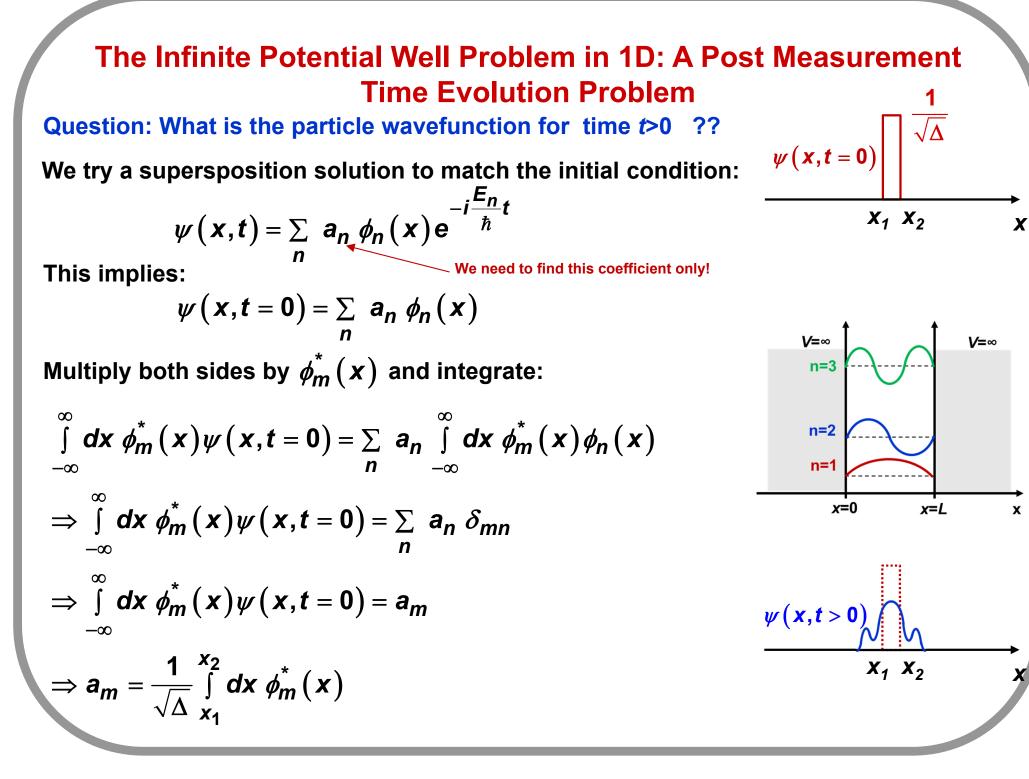


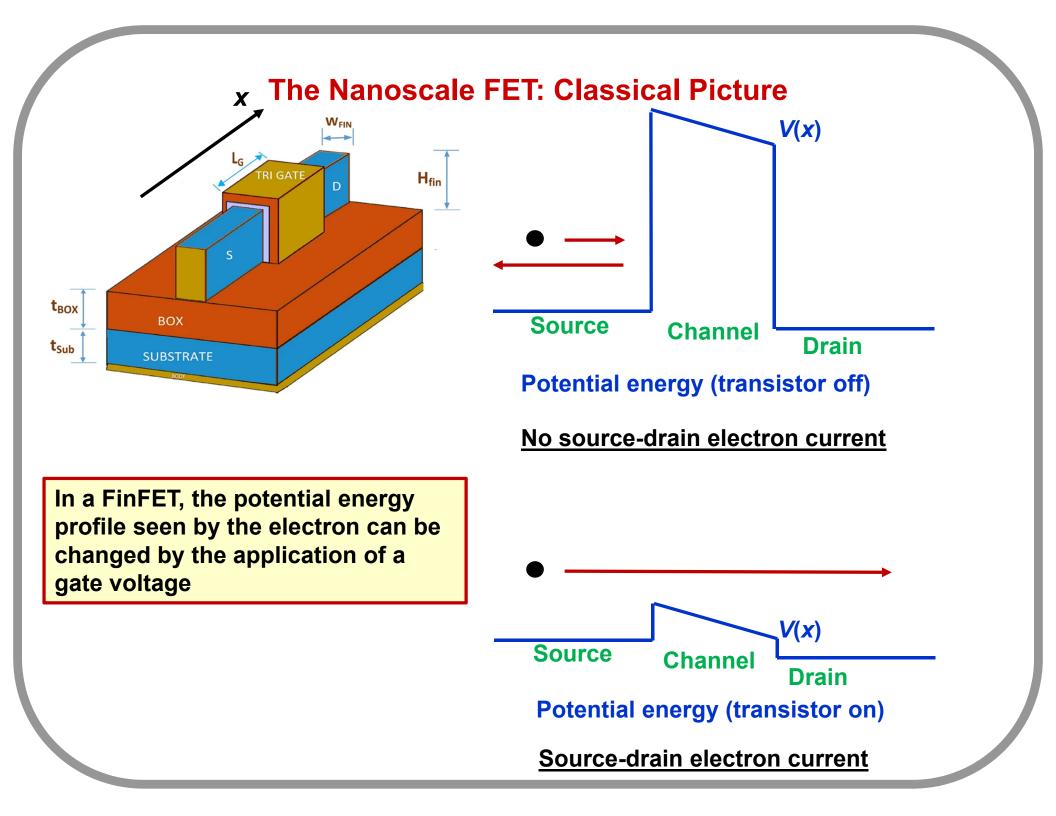
A time *t*=0, a measurement is made to locate the particle

The measurement is not very precise and post-measurement the particle is known to be somewhere inside the dashed region of thickness  $\Delta$ 

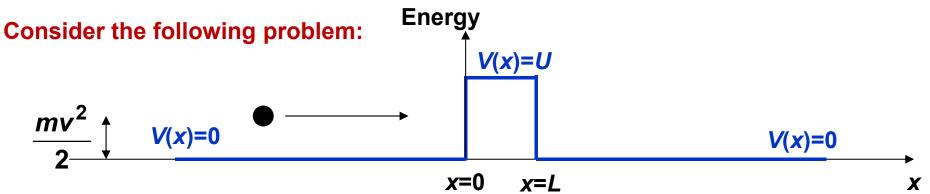
So immediately after the measurement its wavefunction can be taken to be roughly:

$$\psi(x,t=0^{+}) = \begin{cases} \frac{1}{\sqrt{\Delta}} & x_{1} \le x \le x_{2} \\ 0 & \text{otherwise} \end{cases} \xrightarrow{\infty} \int_{-\infty}^{\infty} dx |\psi(x,t=0)|^{2} = 1$$





# **Barrier Tunneling in Quantum Physics**



#### **Classical physics:**

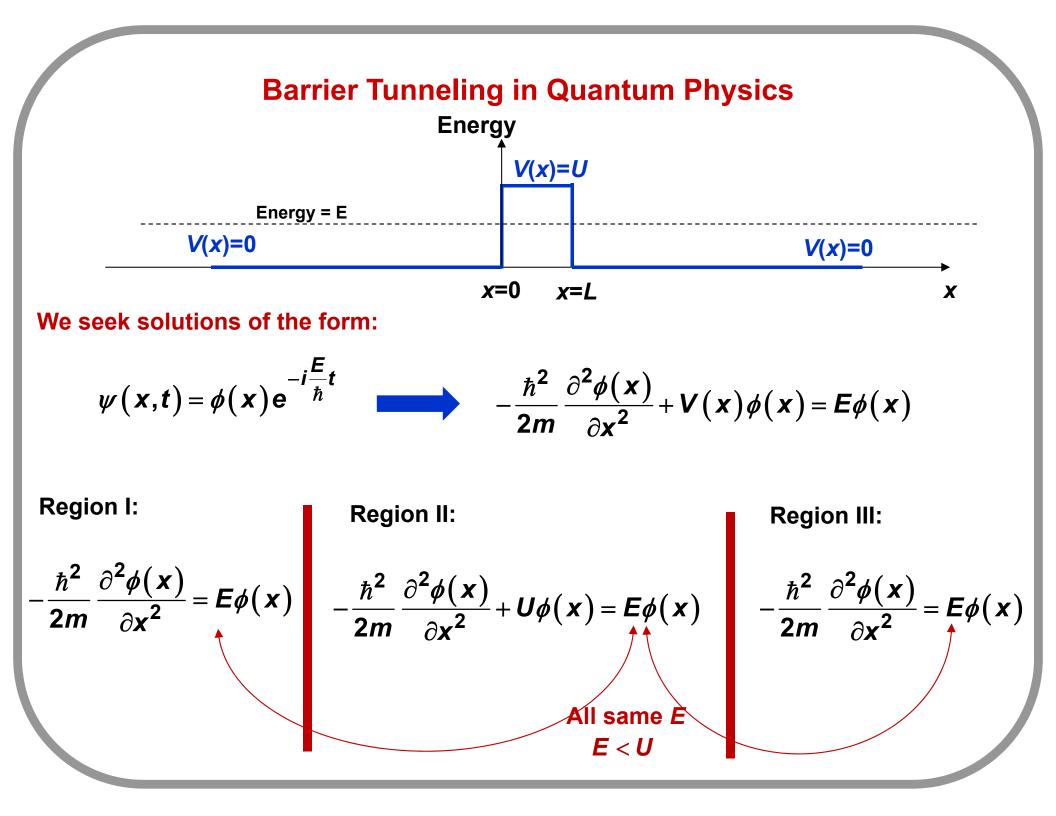
A particle with KE equal to  $mv^2/2$  is coming from the left towards a region where the potential is *U* over a distance *L* 

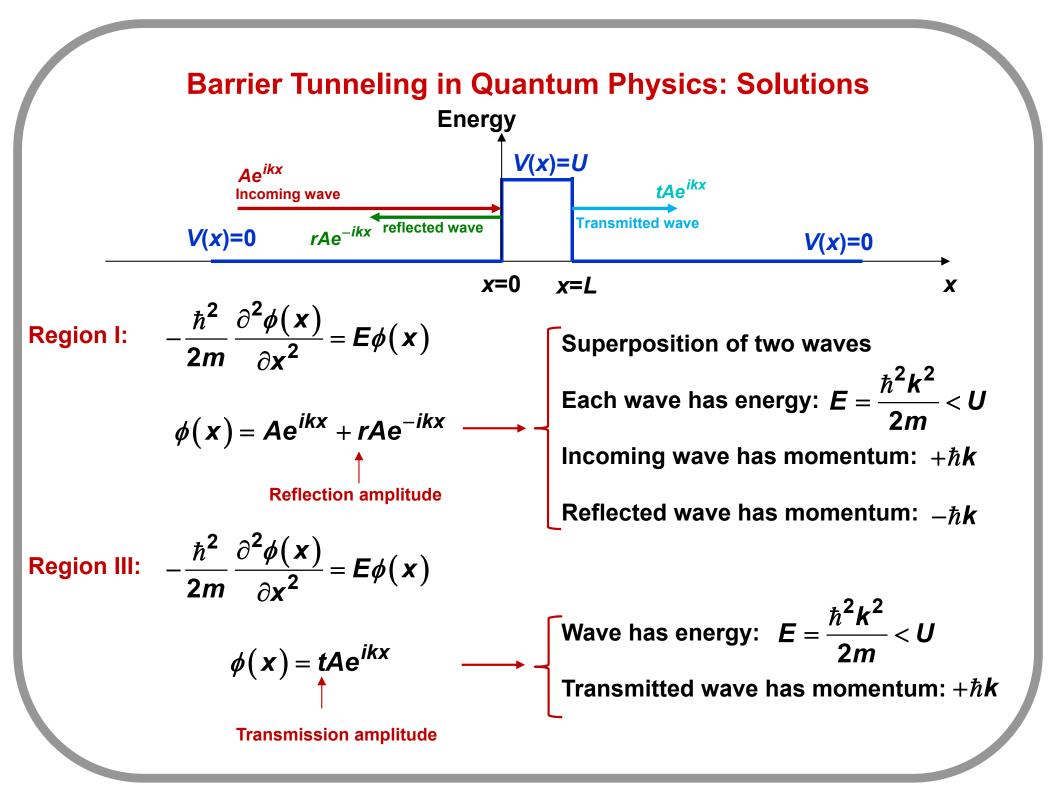
The KE of the particle is less than U:  $E = \frac{mv^2}{2} < U$ 

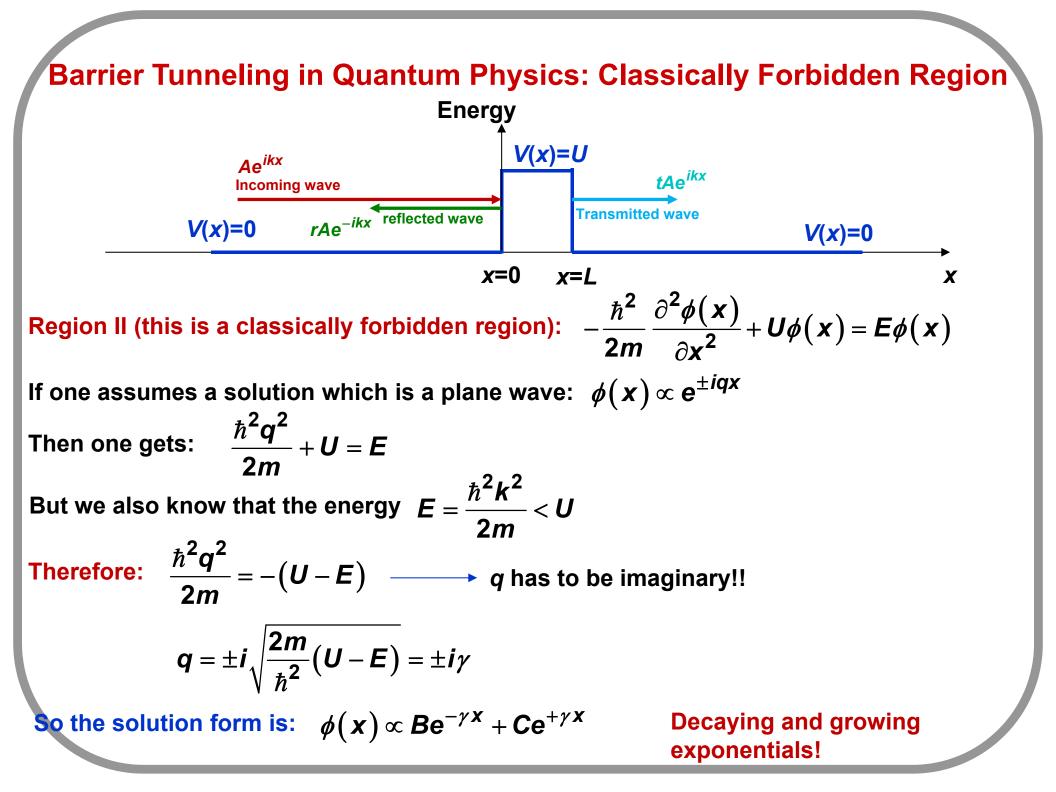
The particle doesn't have enough KE to go through the potential hill, and will therefore bounce back. The potential hill is also called a potential barrier.

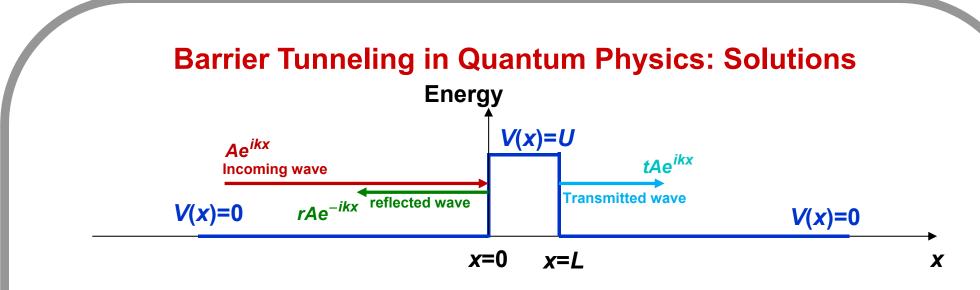
#### **Quantum physics:**

There is a chance that the particle will go through, or tunnel through, the potential barrier and there is a chance that the particle with bounce back!







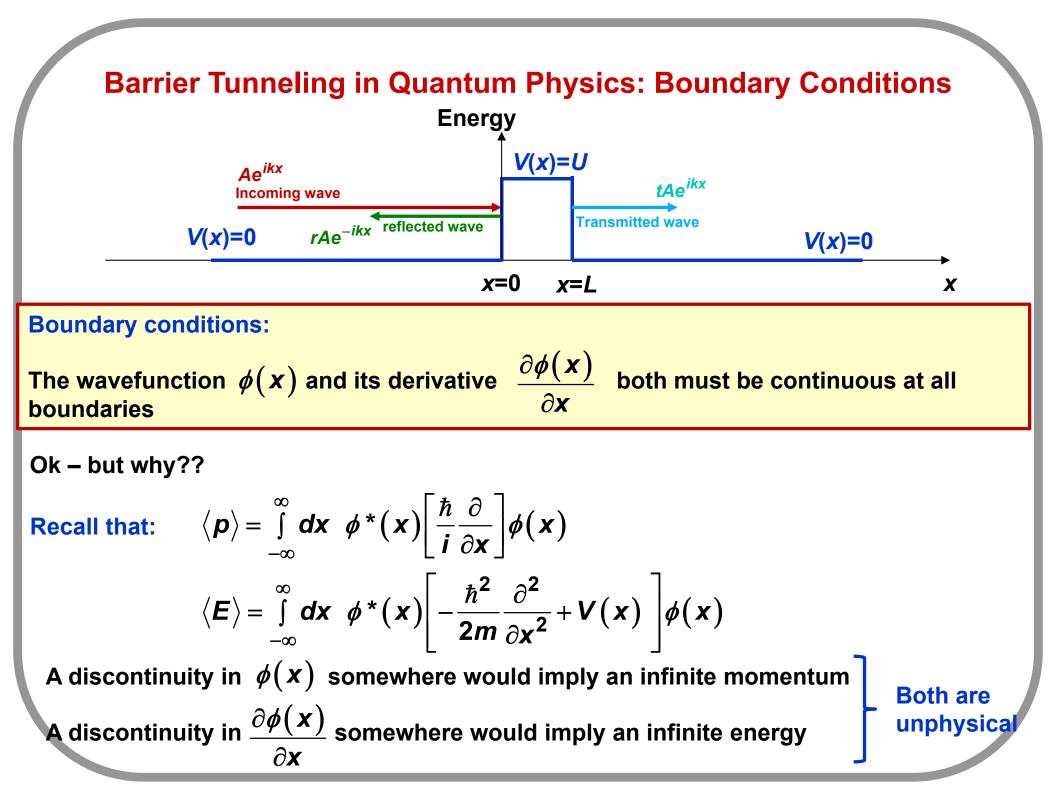


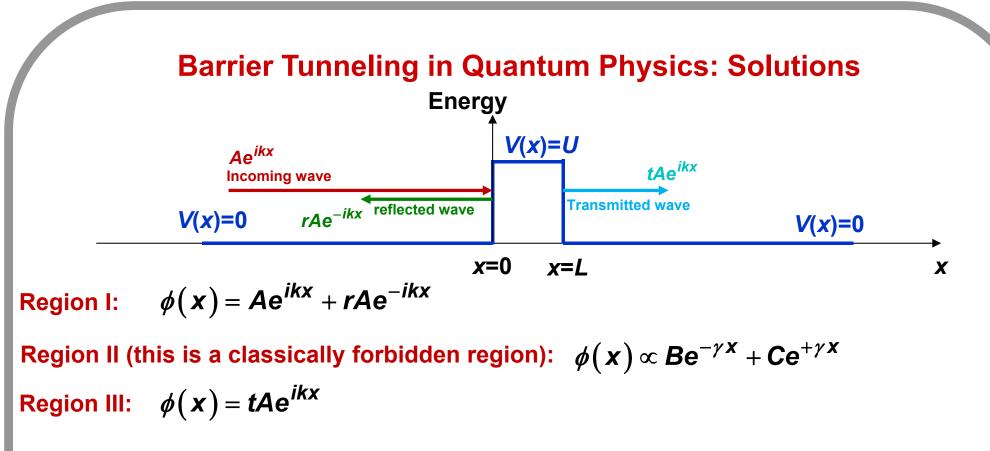
**Region I:**  $\phi(x) = Ae^{ikx} + rAe^{-ikx}$ 

Region II (this is a classically forbidden region):  $\phi(x) \propto Be^{-\gamma x} + Ce^{+\gamma x}$ Region III:  $\phi(x) = tAe^{ikx}$ 

Now we need to stitch together these solutions at the boundaries

We have 4 unknown coefficients, which means we need four boundary conditions!





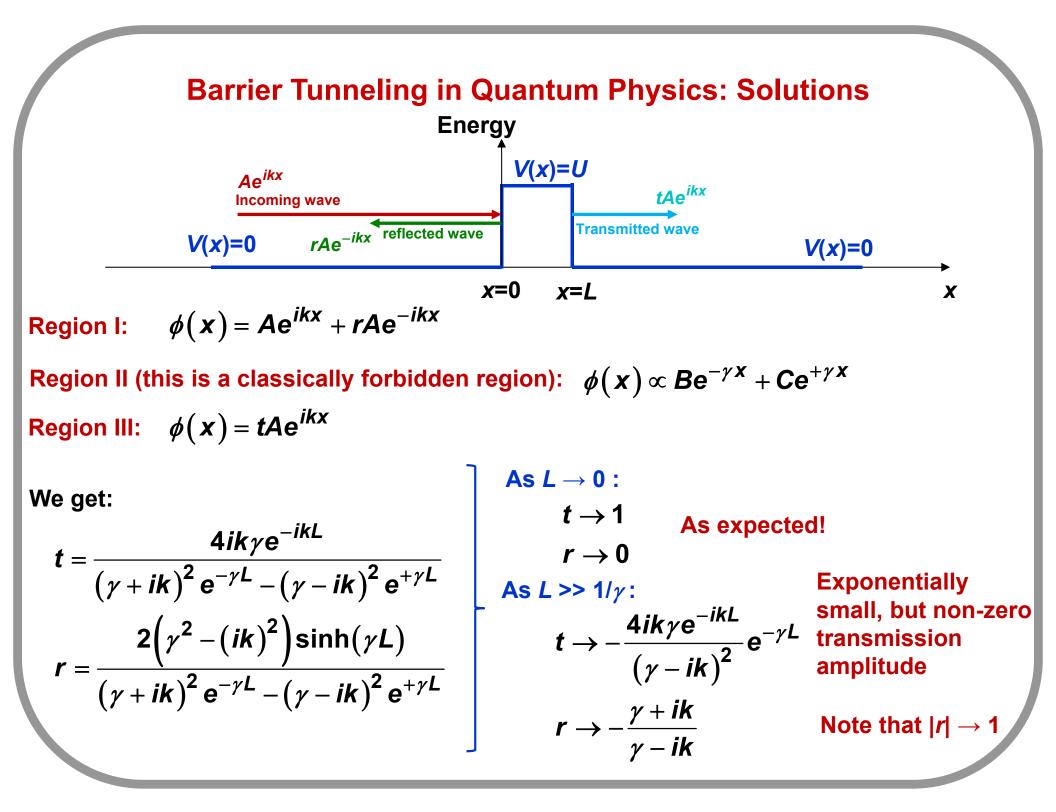
Apply all the boundary conditions:

$$A(1+r) = B + C$$
  

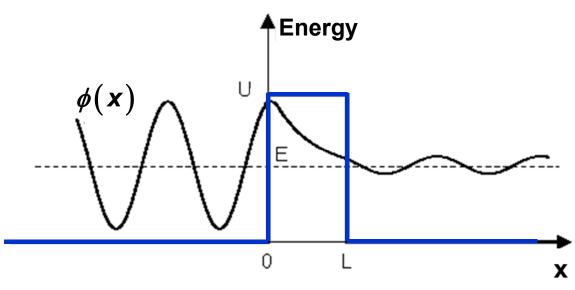
$$ikA(1-r) = -\gamma(B-C)$$
  

$$Be^{-\gamma L} + Ce^{+\gamma L} = tAe^{ikL}$$
  

$$-\gamma (Be^{-\gamma L} - Ce^{+\gamma L}) = iktAe^{ikL}$$



### **Barrier Tunneling in Quantum Physics: Solutions**



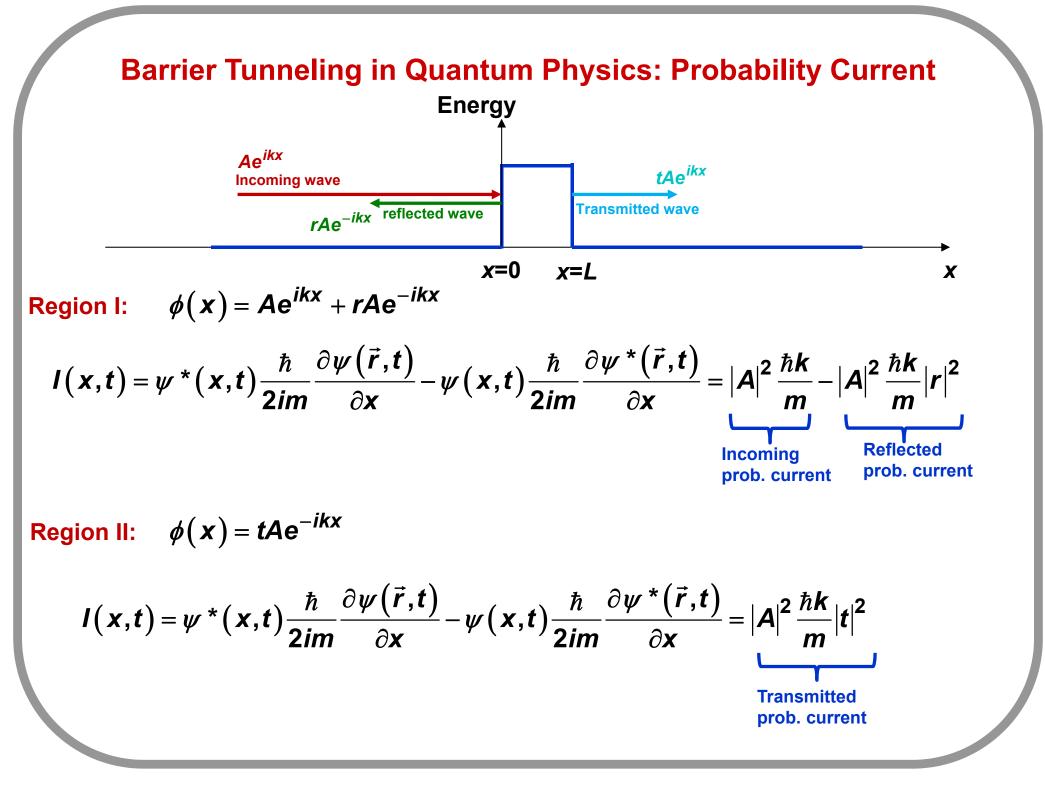
As  $L >> 1/\gamma$ :

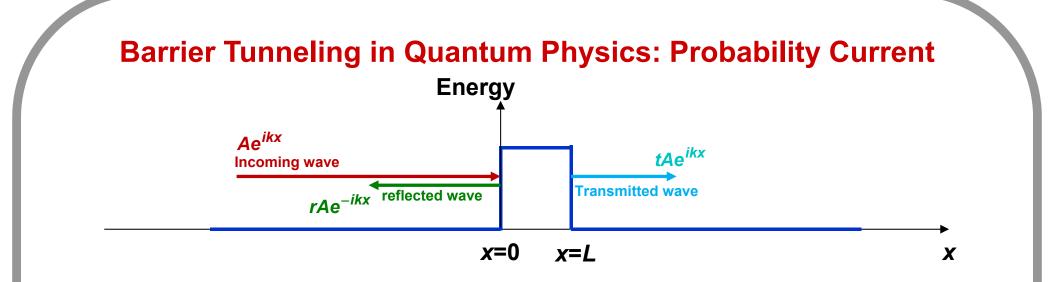
$$t \rightarrow -\frac{4ik\gamma e^{-ikL}}{(\gamma - ik)^2} e^{-\gamma L}$$
$$r \rightarrow -\frac{\gamma + ik}{\gamma - ik}$$

Exponentially small, but non-zero transmission amplitude

Note that  $|\mathbf{r}| \rightarrow 1$ 

$$\boldsymbol{t} \sim \mathbf{e}^{-\gamma L} = \mathbf{e}^{-\sqrt{\frac{2m}{\hbar^2}(\boldsymbol{U}-\boldsymbol{E})}} L$$





**Conservation of probability:** Incoming probability current (coming towards the potential barrier) must equal the outgoing probability current (going away from the potential barrier)

#### This implies:

Incoming probability current = reflected probability current + transmitted probability current

$$|\mathbf{A}|^{2} \frac{\hbar \mathbf{k}}{m} = |\mathbf{A}|^{2} \frac{\hbar \mathbf{k}}{m} |\mathbf{r}|^{2} + |\mathbf{A}|^{2} \frac{\hbar \mathbf{k}}{m} |\mathbf{t}|^{2}$$
$$\Rightarrow \mathbf{1} = |\mathbf{r}|^{2} + |\mathbf{t}|^{2}$$

