# Quantum Mechanics



## Wave function:

- In the last chapter we saw that any particle has both particle- and wave-like properties.

- We saw previously that the functions describing a plane EM-wave is:

$$\vec{E} = E_0 \hat{x} \cos\left(kz - \omega t\right)$$

and the associated intensity(power/area) is proportional to the square of the wave amplitude:

$$I = \frac{1}{\mu_0}\left[E_0^2 \cos^2(kz - \omega t)\right]_{\rm avg}$$

- In this chapter we are interested in answering the question: “What is the wave function for a particle such as the electron in quantum mechanics?”

- To begin we will define the **wave function** of a particle in a single spatial dimension:

$$\Psi(x,t)$$

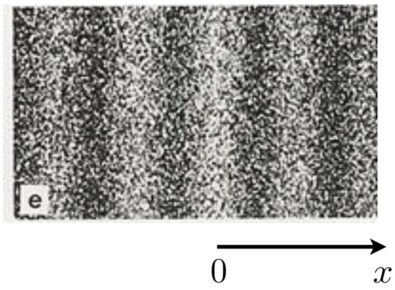
- To understand the physical meaning of the wave function, lets again look at the double slit experiment.

- To start, we will not worry about the time dependence: $\Psi(x,t) \rightarrow \Psi(x)$

- The screen measures the intensity of electrons

- The brighter the screen, the greater the density of electrons hitting that region.

- Since intensity is proportional to the square of the wave amplitude:




$$|\Psi(x)|^2 = P(x)$$

- Here P(x) is the probability <u>of a single</u> electron being found in the region between [x,x+dx]

$$P(x)dx = |\Psi(x)|^2\, dx$$

- We must take the absolute value squared of the wave function since it is a complex-valued function. (It is impossible to measure a probability)

- Because the probability of finding the electron somewhere on the screen is unity, we also have the following condition:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2\, dx = \int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)dx = \int_{-\infty}^{\infty} P(x)dx = 1$$

complex conjugate



- The requirement that P(x)=1 gives us the amplitude of the wave function.

**<u>Momentum:</u>**

- Let us consider a particle that is free to move.

  - The wave function must be a traveling wave since the particle travels.

  - Like the EM-wave, the solution must be sinusoidal

  - Setting t=0 (we are still ignoring time) we have:

$$\Psi(x) = C\cos(kx) + D\sin(kx)$$

or using complex number notation:

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

  - Here A,B,C,D are all complex valued amplitudes and k is the wave number:

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p\frac{2\pi}{h} = \frac{p}{\hbar}$$

  - Thus, the momentum of the particle is given by: $p = \hbar k$

- How do we find the momentum of a particle if we know the wave function?

- Suppose we have the following wave function: $\Psi(x) = Ae^{ikx}$

- To get the momentum from this wave function we want to find a mathematical operation such that

$$\hat{p}\Psi(x) = \hbar k \Psi(x)$$

"hat" means operator

$\hat{p}$ is called the **momentum operator** and is defined to be: $\hat{p} = -i\hbar \frac{d}{dx}$

The momentum operator is proportional to the slope of the wave function

- That this gives the required result $\hbar k$ is shown below:

$$-i\hbar \frac{d\Psi(x)}{dx} = -i\hbar \frac{d}{dx} Ae^{ikx} = -i\hbar A(ik)e^{ikx} = \hbar k Ae^{ikx} = \hbar k \Psi(x)$$

- The wave function $\Psi(x) = Ae^{ikx}$ describes a particle moving to the left with the momentum $p = \hbar k$



- If we used $\Psi(x) = Be^{-ikx}$ then the momentum operator gives $p = -\hbar k$

-> The particle is moving to the left

**Kinetic energy of free particle:**

- Since we are dealing with a free particle we know that the kinetic energy is given classically as $K = p^2/2m$

- Quantum mechanically we can use the momentum operator to get

$$\hat{K} = \hat{p}^2/2m = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

- Applying to the wave function $\Psi(x) = Ae^{ikx}$ :

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) = -ik\frac{\hbar^2}{2m}\frac{d}{dx}Ae^{ikx} = \frac{\hbar^2 k^2}{2m}Ae^{ikx} = \frac{\hbar^2 k^2}{2m}\Psi(x)$$

- So again, we get the correct expression for the kinetic energy of a freely moving particle

## Time-independent Schrödinger equation:

- Suppose we move from a free particle to a particle in a potential U(x), then the equation for the total energy is given by the **time-independent Schrödinger equation**:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + U(x)\Psi(x) = E\Psi(x)}$$

- What are the wave functions that satisfy this equation?

- The wave function must satisfy the following conditions:

I) $\Psi(x)$ must be continuous in space -> the derivative of $\Psi(x)$ must also exist and be finite.

Momentum must be well defined and not infinite

II) $\Psi(x)$ must be zero where the potential $U(x) = \infty$

Cannot find a particle where it takes infinite amounts of energy to put it

III) The amplitude of $\Psi(x)$ must be such that $\int_{-\infty}^{\infty} |\Psi(x)|^2\, dx = 1$

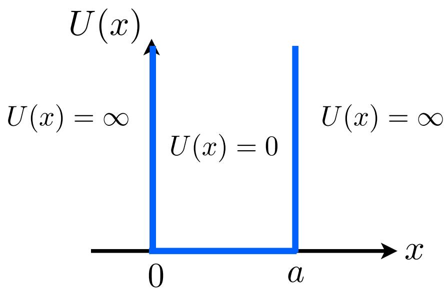
Probabilities must always add up to unity



## Infinite Potential Well:

- Suppose the potential U(x) is given by:

$$U(x) = \begin{cases} \infty : x \leq 0 \\ 0 : x \in (0, a) \\ \infty : x \geq a \end{cases}$$




- Then immediately from rule #2 we know that the wave function satisfies: $\Psi(0) = \Psi(a) = 0$

- These **boundary conditions** will determine the shape of the wave functions

- Taking the general form of the wave function $\Psi(x) = C\cos(kx) + D\sin(kx)$

- Since $\Psi(0) = 0$ we have $\Psi(0) = C\cos(0) + D\sin(0)$

$$C = 0$$

- Using $\Psi(a) = 0$ we have $\Psi(a) = D\sin(ka) = 0$

$$ka = \frac{2\pi a}{\lambda} = n\pi, \quad n = 1, 2, \ldots$$

(n=0 -> wavelength = infinity which does not work)

- Therefore only certain wavelengths are allowed inside the potential well:

$$\lambda_n = \frac{2a}{n}, \quad n = 1, 2, \ldots$$

- The solution to the wave function is thus:

$$\Psi(x) = \begin{cases} 0 & : x \leq 0 \\ D \sin\left(\frac{n\pi x}{a}\right), n = 1, 2, \ldots & : x \in (0, a) \\ 0 & : x \geq a \end{cases}$$

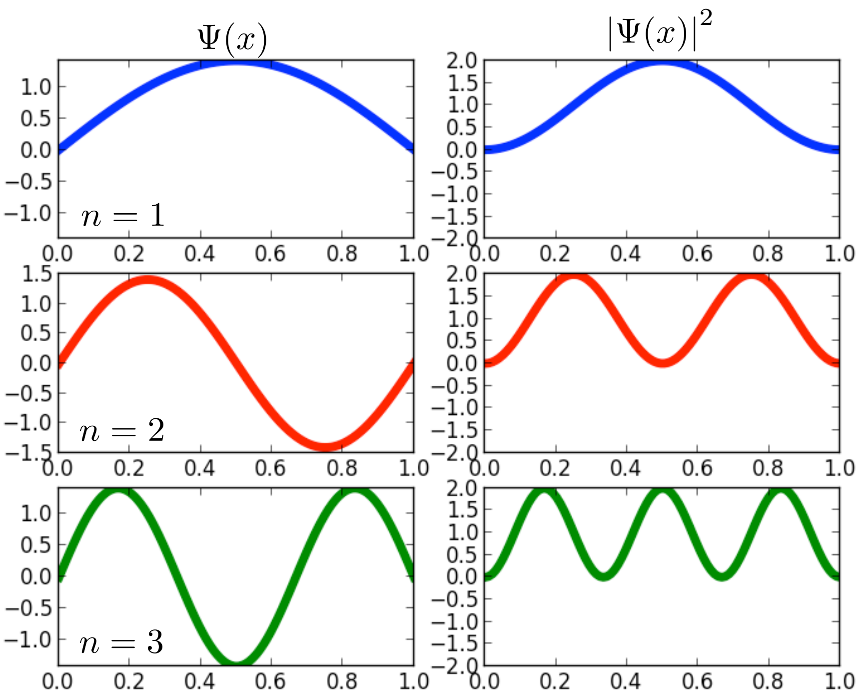
- Rule #3 also tells us that that amplitude D must give unit probability:

$$1 = \int_0^a |\Psi(x)|^2 \, dx = \int_0^a \left| D \sin\left(\frac{n\pi x}{a}\right)\right|^2 dx = |D|^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = |D|^2 \frac{a}{2}$$

$$D = \sqrt{\frac{2}{a}} e^{i\theta}$$ ( Can set $\theta = 0$ in general)

$$\boxed{\Psi(x) = \begin{cases} 0 & : x \leq 0 \\ \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, \ldots & : x \in (0, a) \\ 0 & : x \geq a \end{cases}}$$



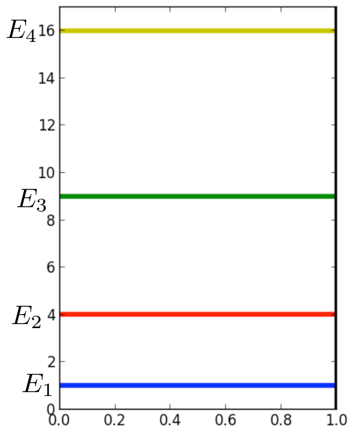


- We can also compute the energy for each different n-state which we call $E_n$ :

$$E_n \Psi_n(x) = -\frac{\hbar^2}{2m}\frac{d^2\Psi_n(x)}{dx^2} = -\frac{\hbar^2}{2m}\frac{n\pi}{a}\frac{d}{dx}\left(\sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right)\right)$$

$$= \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \Psi_n(x)$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$




- The energy goes as the square of the index "n"

- Energies lower than the height of the potential well are called **bound states**

- The infinite potential box has an infinite number of bound states



- What about more than one dimension?

- If the potential is separable, $U(x,y) = U(x)U(y)$ then the wave function is also separable

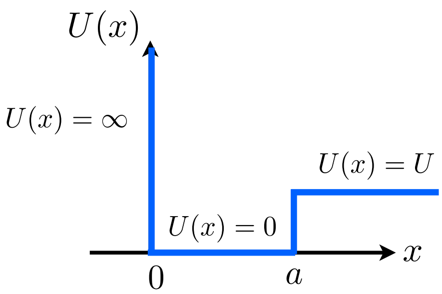
$$\Psi(x,y) = \Psi(x)\Psi(y)$$

- We can solve for each direction separately, exactly like the 1D example

**<u>Finite Potential Well:</u>**

- Suppose we now have a potential well that is finite on one side:

$$U(x) = \begin{cases} \infty : x \leq 0 & \text{Region \#1} \\ 0 : x \in (0,a) & \text{Region \#2} \\ U : x \geq a & \text{Region \#3} \end{cases}$$




- Solve for the wave function in each section alone and then combine using boundary conditions

- In Region #1 we still have: $\Psi(x) = 0$

- In Region #2 we have: $\Psi(x) = D\sin(kx)$ since $\Psi(0) = 0$ still

- In Region #3:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + U\Psi(x) = E\Psi(x) \quad \Rightarrow \quad \frac{d^2\Psi(x)}{dx^2} = \frac{2m}{\hbar^2}(U-E)\Psi(x)$$

Case #1: E>U:

$$\frac{2m}{\hbar^2}(U-E) < 0 \quad \Rightarrow$$ - Solutions still oscillate, but with different wavenumber

$$\Psi(x) = E\cos(k'x) + F\sin(k'x)$$

- Inside region #2: $E = \frac{\hbar^2 k^2}{2m}$ - Inside region #3: $E - U = \frac{\hbar^2 k'^2}{2m}$

$$\Rightarrow \quad k' = \sqrt{k^2 - \frac{2mU}{\hbar^2}}$$

- Wavenumber is smaller (Wavelength larger) in Region #3 if E>U



- The wave function in all three regions is therefore:

$$\Psi(x) = \begin{cases} 0 : x \leq 0 \\ D\sin(kx) : x \in (0,a) \\ E\cos(k'x) + F\sin(k'x) : x \geq a \end{cases}$$

- We can find D,E,F by using the boundary conditions and probability conservation:

  - Wave function at x=a is continuous
  - Derivative of wave function at x=a is continuous
  - Amplitude must satisfy probability =1

3 conditions, 3 unknowns

Case #2: E<U:

$$\frac{2m}{\hbar^2}(U-E) > 0 \quad \Rightarrow$$ - Solutions are exponentials

- let $\gamma^2 = \frac{2m}{\hbar^2}(U-E)$ then solution to wave equation in Region #3 is:

$$\Psi(x) = Fe^{-\gamma x} + Ge^{\gamma x}$$

- In order for probability to equal 1, we must set G=0

$$\Rightarrow \quad \Psi(x) = Fe^{-\gamma x}$$ (Decaying exponential)

- Unlike classical physics, the wave function is not zero when U>E, and there is a non-zero probability of finding the particle in the classically forbidden Region #2

- If E<U, then the wave function always decays exponentially in that region.

- The solution in all regions is:

$$\Psi(x) = \begin{cases} 0 : x \leq 0 \\ D\sin(kx) : x \in (0,a) \\ Fe^{-\gamma x} : x \geq a \end{cases}$$

- The last two coefficients D & F are found from wav function and its derivative at x=a

- The decay rate $\gamma$ is related to the wavenumber via:

$$k = \frac{2m}{\hbar^2}(U-E) = \frac{2mU}{\hbar^2} - \frac{2mE}{\hbar^2} = \frac{2mU}{\hbar^2} - k^2$$

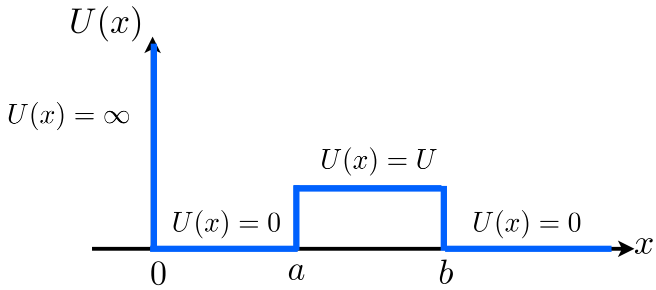


**Tunneling:**

- If there is a non-zero chance of finding a particle in the classically forbidden region E<U, then can a particle actually go through a barrier of finite width?

-Suppose we have the potential:

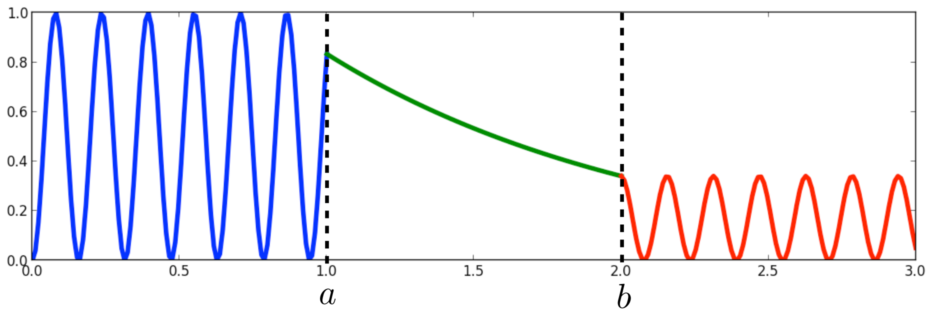
$$U(x) = \begin{cases} \infty : x \leq 0 \\ 0 : x \in (0,a) \\ U : x \in [a,b] \\ 0 : x \geq b \end{cases}$$




- We have already calculated what the wave function is in each separate region:

$$\Psi(x) = \begin{cases} 0 : x \leq 0 \\ D\sin(kx) : x \in (0,a) \\ Fe^{-\gamma x} : x \in [a,b] \\ G\sin(kx+\phi) : x \geq b \end{cases}$$

In general, there will be a phase shift since LHS is no longer infinite potential




- If the amplitude of the wave function does not decay to zero inside the forbidden region (E<U), then the amplitude for x>b must also be non-zero since the boundary conditions must match at x=b.

➡ - There is a non-zero probability of the particle being found on the other side of the barrier x>b

- This is called **Tunneling,** and it is impossible in classical physics

- The probability that a particle on the left will appear on the right of the barrier is called the **transmission amplitude** and it is given by:

$$\boxed{T = \frac{|\Psi(b)|^2}{|\Psi(a)|^2} = \frac{|Fe^{-\gamma b}|^2}{|Fe^{-\gamma a}|^2} = \left|e^{-\gamma(b-a)}\right|^2 = e^{-2\gamma(b-a)}}$$

- Transmission decays exponentially with barrier width.