PH 112: Quantum Physics and Applications

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Week 03 Lecture 3: Wave function interpretation and properties

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Schrodinger Equation: Recap

- Erwin Schrodinger proposed equation to describe the time and position dependence of the matter waves:

Time-dependent Schrodinger equation

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

$$\Psi(x,t)=\psi(x)T(t)$$

For time-independent potentials

Time independent Schrodinger Eq (TISE)

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

Question: How to interpret $\Psi(x,t) and\ \psi(x)$?

Classical wave solutions satisfy?

Solutions of Schrodinger Equation

Question: Whether the solutions of classical wave equation are also solutions to Schrodinger equation?

$$\Psi(x,t) = A\sin(kx - \omega t)$$

Answer: No

Proof:

$$\frac{\partial \Psi}{\partial t} = -\omega A\cos(kx - \omega t)$$

$$\frac{\partial \Psi}{\partial x} = kA\cos(kx - \omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A^2 \cos(kx - \omega t)$$

$$-i\hbar\omega A\cos(kx - \omega t) \neq \left(\frac{\hbar^2 k^2}{2m} + V\right) A\sin(kx - \omega t)$$

Solutions of Schrodinger Equation

Question: What about $\Psi(x,t) = A\exp\left(i[kx-\omega t]\right)$? Answer: Yes

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx-\omega t)}$$

$$\frac{\partial \Psi}{\partial x} = ikAe^{i(kx-\omega t)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx-\omega t)}$$

$$-i\hbar(i\omega) = \left(\frac{\hbar^2 k^2}{2m} + V\right)$$

$$E = \frac{p^2}{2m} + V$$

The solution is complex!

$\Rightarrow \Psi(x,t)$ *cannot* be a physical wave (e.g. electromagnetic waves).

How to relate $\Psi(x,t)$ to measurements on a system?

Solutions and Uncertainty principle

Example 1: Free Particle

For a free particle $V(x) = 0$ and TISE is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

and has solutions

$$\psi = e^{ikx} \quad or \quad e^{-ikx} \qquad where \qquad E = \frac{k^2\hbar^2}{2m}$$

Thus the solution to the time-dependent Schrödinger equation is:

$$\Psi(x,t) = \psi(x)\,T(t) = e^{i(\pm kx - Et/\hbar)}$$

Corresponds to waves travelling in either $\pm x$ direction with:

(i) an angular frequency, $\omega = E/\hbar \Rightarrow E = \hbar\,\omega$! Corresponding to fixed Energy

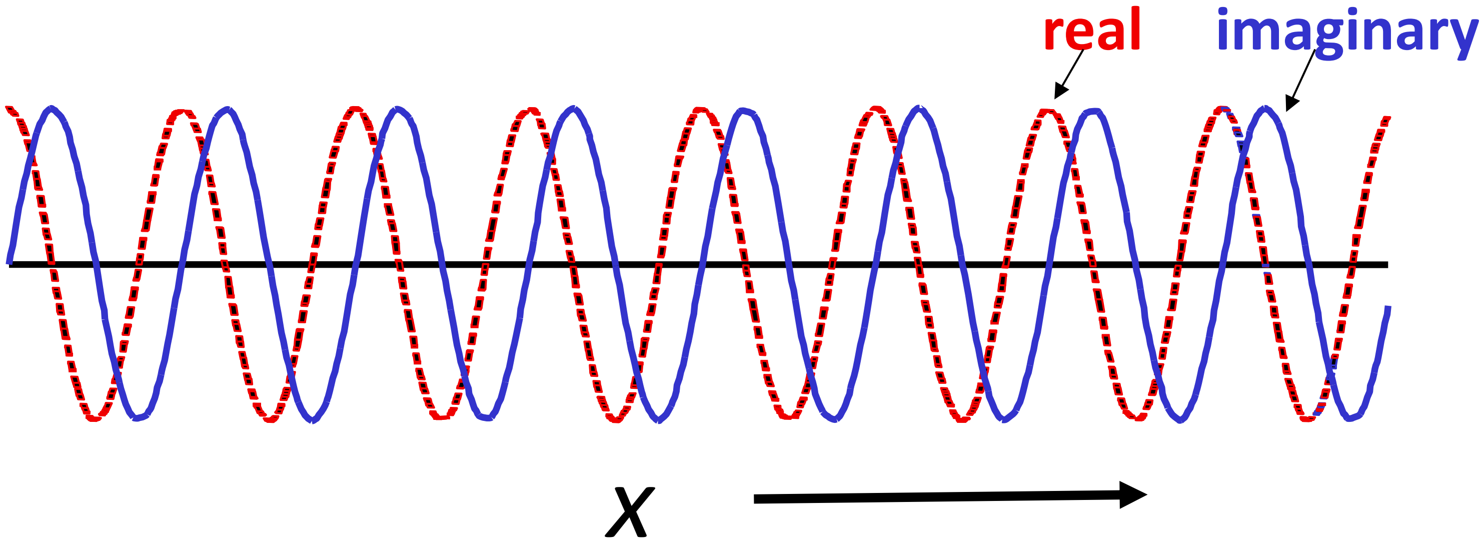
(ii) a wave-number, $k = (2mE)^{1/2}/\hbar = p/\hbar \Rightarrow p = h/\lambda$! Corresponding to fixed momentum

WAVE-PARTICLE DUALITY!

Example 1: Free Particle

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} = \frac{1}{\sqrt{2\pi}} (\cos(kx) + i\sin(kx)) \quad p = \hbar k$$

What is the particle's location in space?



Not localized
$\Longrightarrow$ Spread all over the space!

Position not defined.
Momentum is precisely defined.

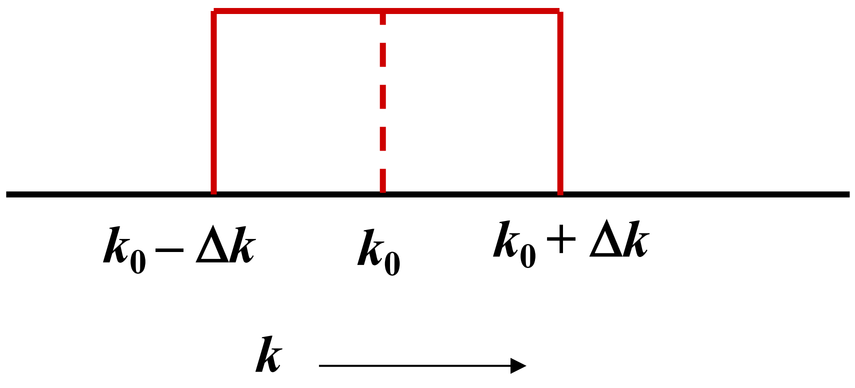
$$\Delta x \to \infty \quad \Delta p \to 0$$

Example 2: Square wave packet

- If $\Psi(x,t) = Ae^{i(kx-\omega t)}$ is a solution to Schrodinger equation, any superposition of such waves is also a solution:

$$\Psi(x,t) = \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk$$

$$\boldsymbol{k = p/\hbar}$$



Consider wave vectors of equal amplitude in the range $\boldsymbol{k_0 - \Delta k}$ **to** $\boldsymbol{k_0 + \Delta k}$**.**

Out side this range, amplitude = 0. Also, $\boldsymbol{\Delta k \ll k_0}$

Superposition of momentum eigenfunctions

$$\psi_{\Delta k}(x) = \int_{k_0 - \Delta k}^{k_0 + \Delta k} e^{ikx} dk$$

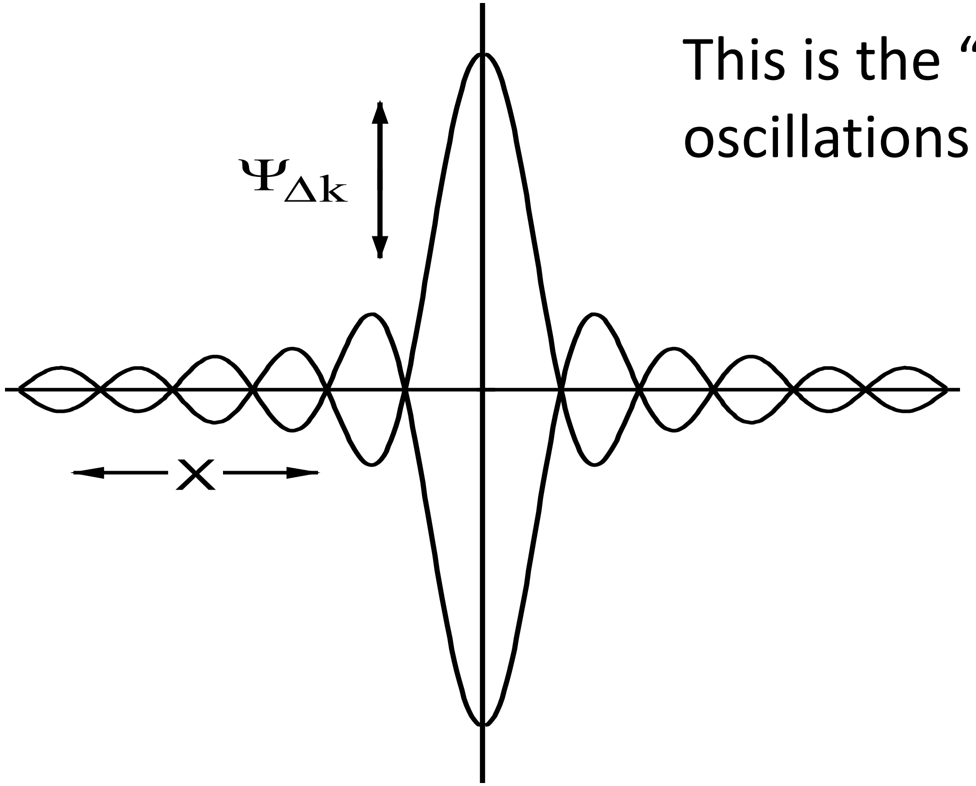
$$\psi_{\Delta k}(x) = \frac{2 \sin \Delta k x}{x} e^{ik_0 x}$$

Integrate over *k* about k_0

Rapid oscillations in envelope of slow, decaying oscillations.

Example 2: Square wave packet

Rewriting we have $$\psi_{\Delta k}(x) = \frac{2\sin\Delta k x}{x}\left[\cos(k_0 x) + i\sin(k_0 x)\right] \qquad \Delta k \ll k_0$$



This is the “envelope.” Real and imaginary parts has rapid oscillations at frequency k_0.

1. The wave packet is “localized” in space.

   As $|x| \to \infty, \psi_{\Delta k}(x) \to 0$

2. Large Δk $\Longrightarrow$ more localized.

3. Large uncertainty in p $\Longrightarrow$ small uncertainty in x

Wavefunction: Definition

- Schrodinger equation dictates the wave function $\Psi(t, x)$.

- At a given time, $\Psi(t, x)$ tells how a particle is distributed through space like a classical wave.

- $\Psi(t, x)$ is the quantum state of an isolated system of one or more particles. $\Psi(t, x)$ contains all the information about the entire system, not a separate wave function for each particle in the system.

  Example: For Hydrogen atom, there is only one wave function. There is no separate $\Psi(t, x)$ for Proton and electron!

Solutions of Schrodinger Equation: Recap

- Solutions of Classical wave equation are not solutions to Schrödinger equation.
- Solutions to Schrödinger equation are complex.
- Solutions satisfy the Heisenberg Uncertainty principle:

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$$

- Key question: Measurements we make will only give real values.

How to interpret complex solutions?

How to interpret complex solutions?

Mathematical detour

- Schrodinger Eq. and its complex conjugate are (assume V(x) is real)

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

$$-i\hbar\frac{\partial\Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + V(x)\Psi^*$$

- Multiply the first equation by Ψ^* and the second equation by Ψ

$$i\hbar\frac{\partial\Psi}{\partial t}\Psi^* = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}\Psi^* + V(x)|\Psi|^2$$

$$-i\hbar\frac{\partial\Psi^*}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi + V(x)|\Psi|^2$$

- Take difference between the two expressions

Mathematical detour

$$i\hbar\left(\frac{\partial\Psi}{\partial t}\Psi^* + \frac{\partial\Psi^*}{\partial t}\Psi\right) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\Psi^* - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)$$

- Simplifying, we get

$$i\hbar\frac{\partial|\Psi|^2}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\frac{\partial\Psi}{\partial x}\Psi^* - \frac{\partial\Psi^*}{\partial x}\Psi\right)$$

- Integrating over x

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty} = 0$$

- If $|\Psi|^2$ is finite at some *t = 0*, it stays the same for all future time.

$\implies |\Psi|^2$ may be a physical relevant quantity compared to Ψ

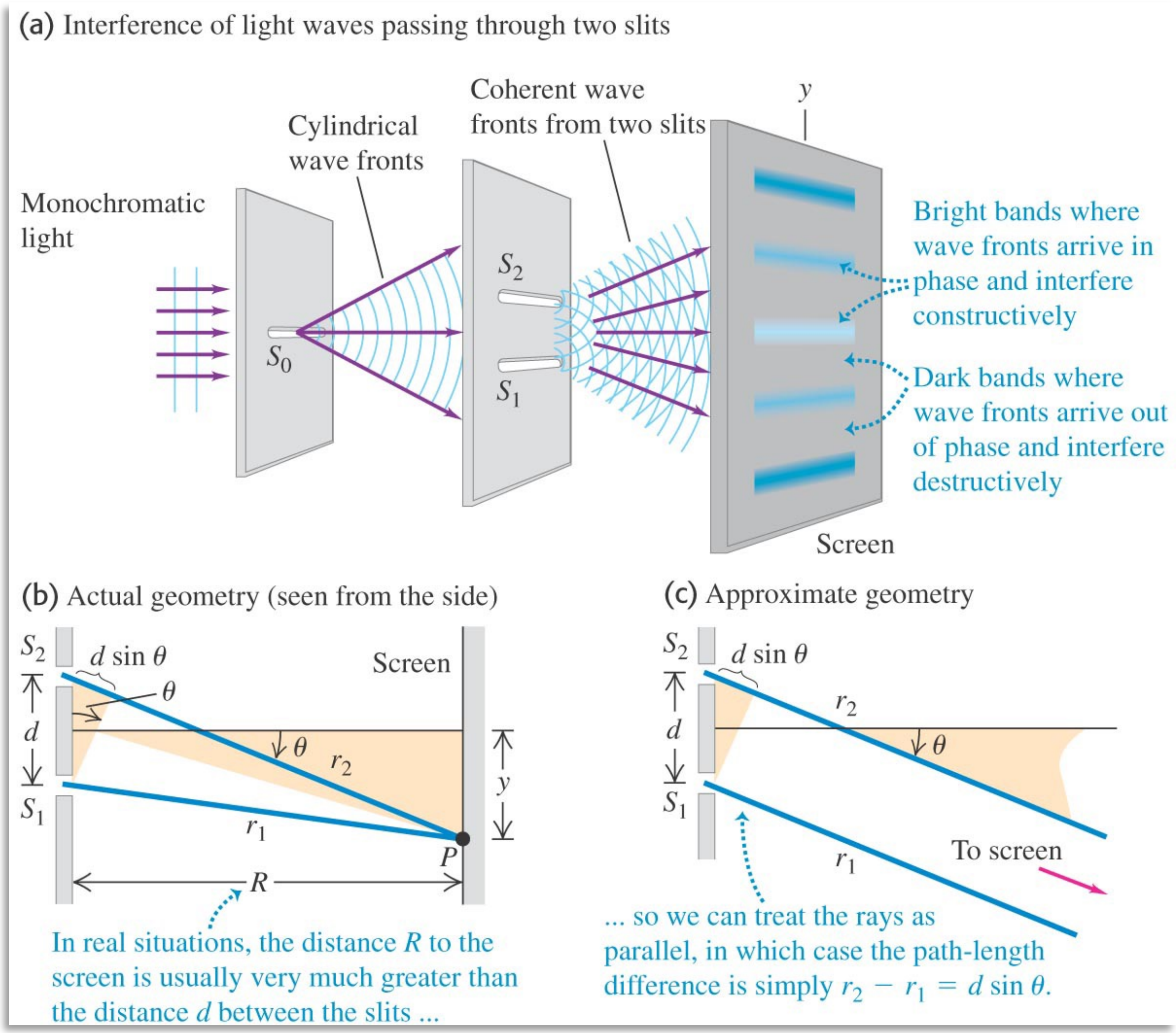
Young's double slit experiment

$$d \sin\theta = m\lambda \quad \text{(in phase, constructive)}$$

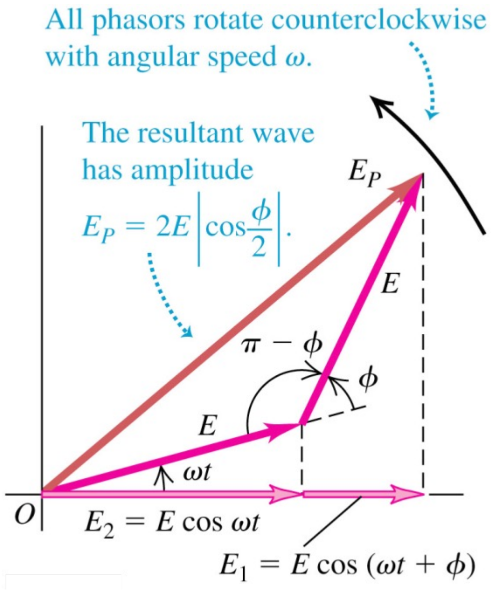
$$d \sin\theta = \left(m + \tfrac{1}{2}\right)\lambda \quad \text{(out of phase, destructive)}$$

By measuring the intensity of the light, we know that some region is dark and some region is bright!

How to calculate the intensity in the interference patterns?



Intensity in interference patterns



- Consider two interfering waves with phase different by phase angle ϕ

$$E_1(t) = E\cos(\omega t + \phi), E_2(t) = E\cos(\omega t)$$

- The resultant wave is the superposition of two waves:

$$E_P \cos\omega t = E\cos(\omega t + \phi) + E\cos(\omega t)$$

- Intensity is related to square of the electric field

$$I = \frac{\varepsilon_0 c E_P^2}{2} = 2\varepsilon_0 c E^2 \cos^2\left(\frac{\phi}{2}\right)$$

$$E_P^2 = E^2 + E^2 - 2E^2\cos(\pi - \phi)$$
$$= E^2 + E^2 + 2E^2\cos\phi = 2E^2(1 + \cos\phi)$$

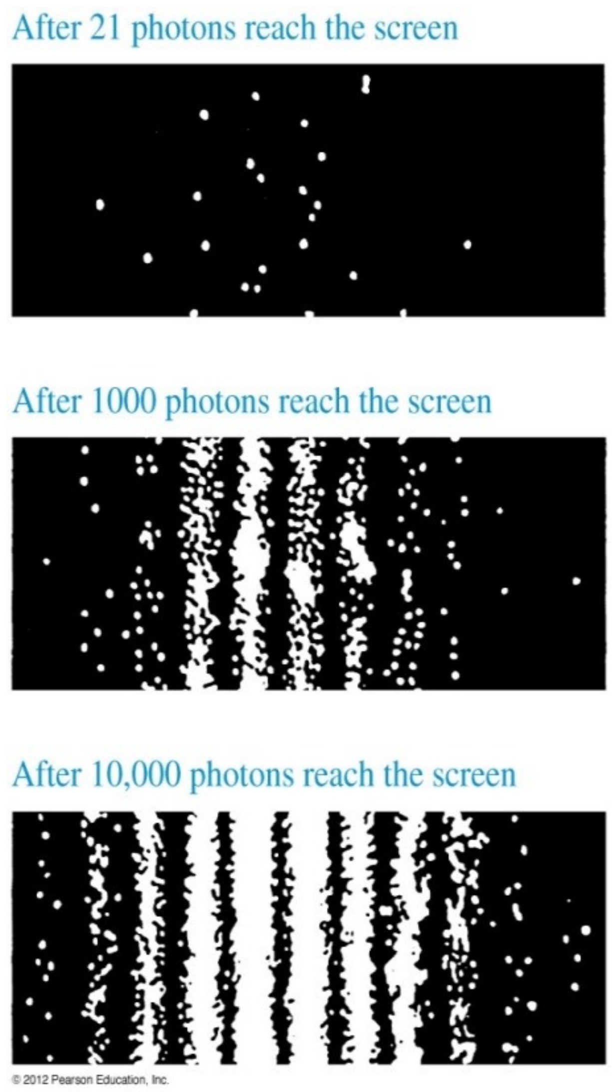
- Using the law of cosines, we have:

$$E_P^2 = 4E^2\cos^2\left(\frac{\phi}{2}\right)$$

Interference intensity pattern corresponds to the square of the electric field!

Understanding Interference from Photon picture

- Interference intensity pattern is the square of the electric field!
- Individual photons land on a screen with a probability given by the intensity pattern.
- The higher intensity regions correspond to higher probability of photons reaching at those points! Or More land where the intensity is high, fewer land where it is low.



Thought experiment with electrons

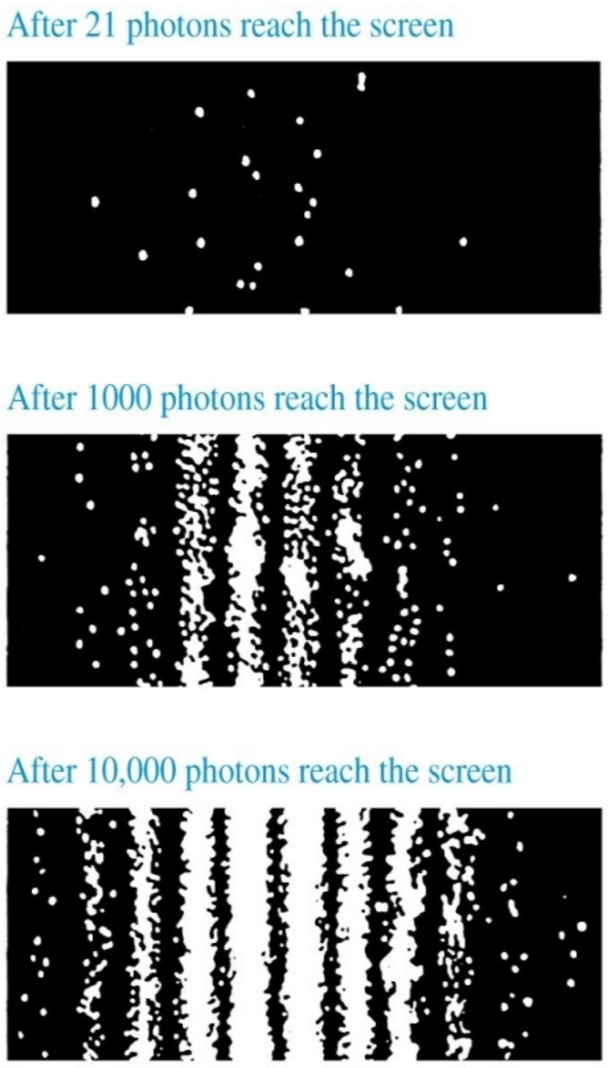
Replace photons with electrons

- Let us do a thought experiment, replace photons with electrons.

- Since electrons also behave as waves, we should be able to see interference pattern in a corresponding double slit experiment.

- In particle picture, individual electrons land on a screen with a probability. More electrons land where the probability is high, fewer land where it is low.

- What quantity can be associated to probability?



How to interpret complex solutions?

- $\Psi(x,t)$ is a scalar function and represents a distribution of “something” in space and time.

- However, any measurable quantity, must be real.

- Born made analogy with the wave theory of light (square of the amplitude can be interpreted as intensity $\Longrightarrow$ finding probability of photons)

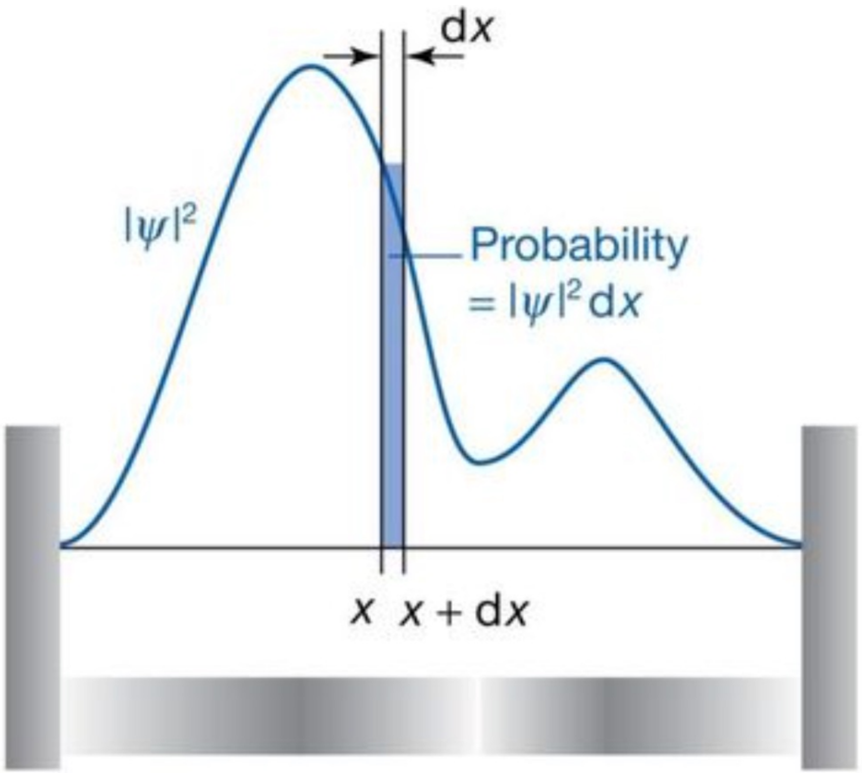
- Similarly, the quantity $$|\Psi(x,t)|^2 = \Psi(x,t)\Psi^*(x,t)$$

  is a real function in space and time.

How to interpret complex solutions?

If the wavefunction of a particle has Ψ at some point x, then the probability of finding the particle between x and x+dx is proportional to

$$\Psi^*(x,t)\Psi(x,t)dx = \left|\Psi(x,t)\right|^2 dx = P(x,t)dx$$



- Wave function contains all the information about a system.

Wave function $\Leftrightarrow$ Classical trajectory

(Quantum) (Newtonian)

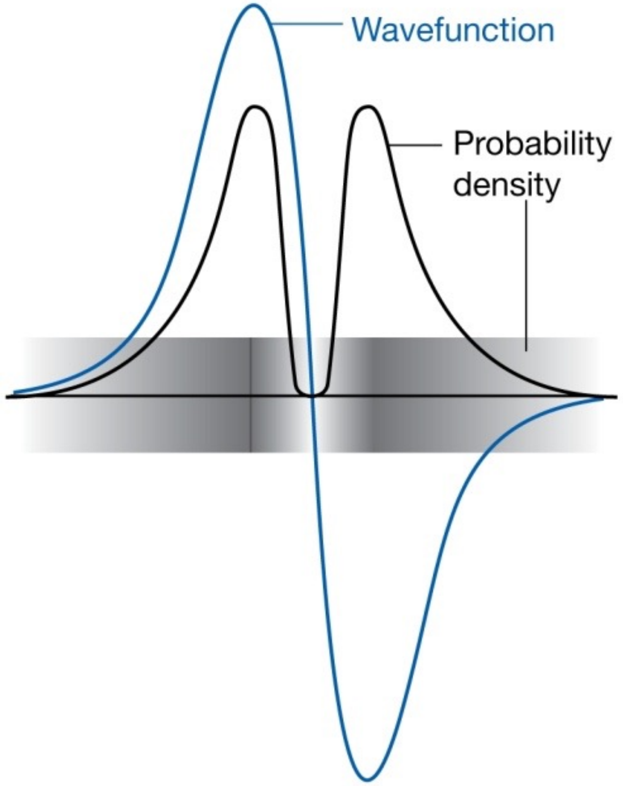
Properties of the wave function

Implications of Born's Interpretation

1. Positivity: $P(x) \geq 0$

   a. The sign of a wavefunction has no direct physical significance.

   b. The positive and negative regions of $\Psi(t, x)$ both correspond to the same probability distribution.



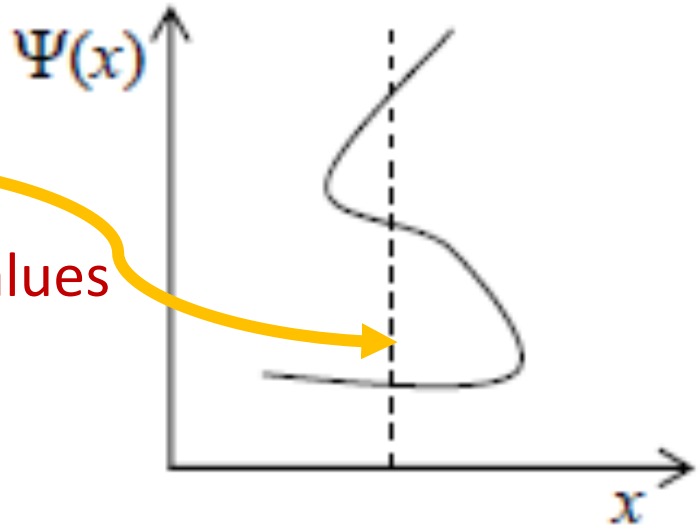
2. Normalization:

$$\boxed{\int_{-\infty}^{\infty} P(x, t_0) dx = \int_{-\infty}^{\infty} |\Psi(x, t_0)|^2 dx = 1}$$

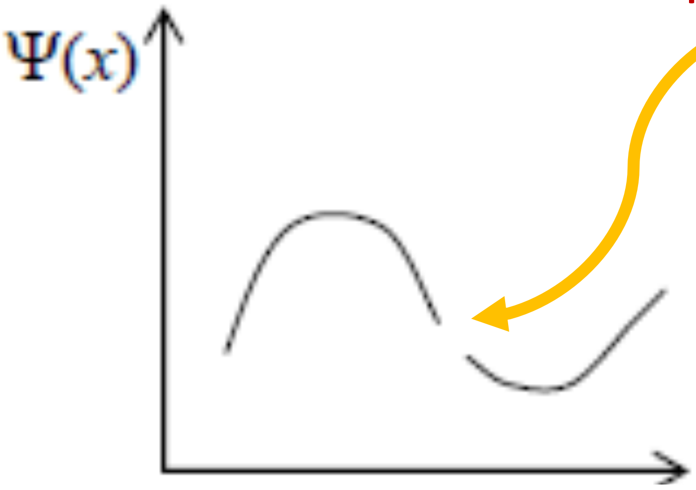
The probability of finding the particle in the universe is 1.

Which of the following Ψ are acceptable?

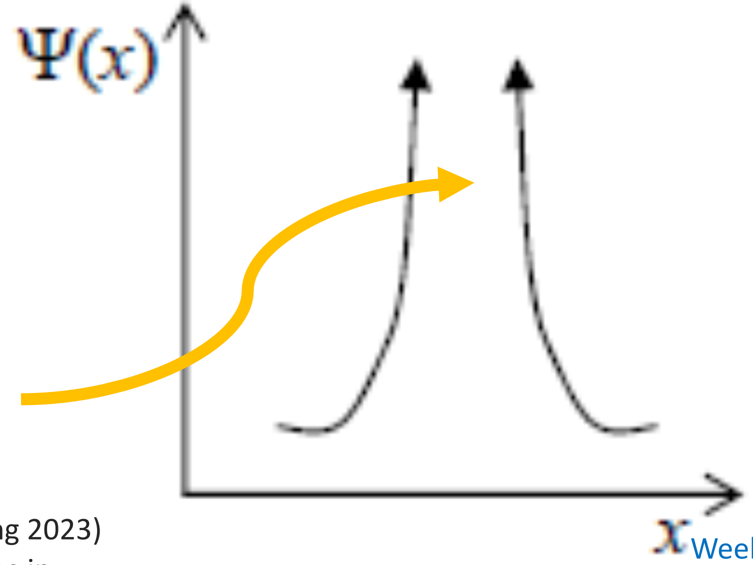
Multiple Ψ values for same x.



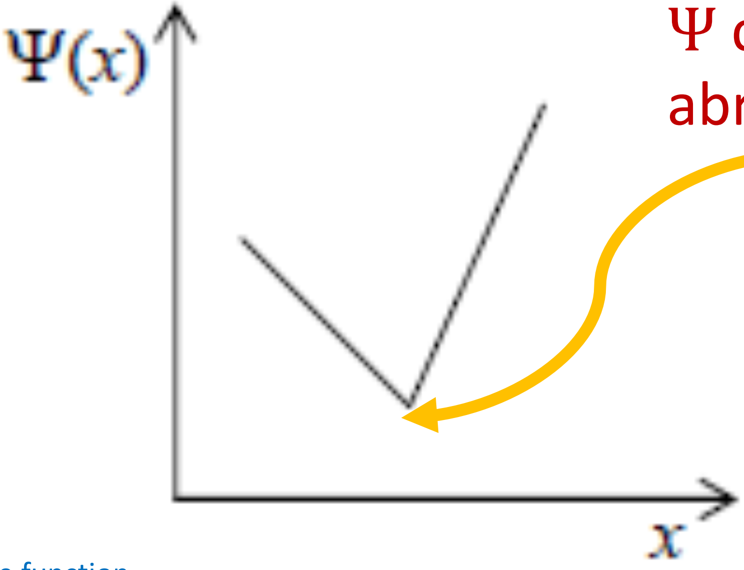
For some x, Ψ is not continuous.



Ψ diverges for some x.



Ψ changes abruptly at some x



Physically acceptable form of wave functions

Finite for all x and t	Probability to find a particle is finite.
Single valued	A single value for the probability of the system being in a given state!
Square integrable	Integral of $\|\Psi\|^2$ over all space must be finite. Hence, total probability is always unity.
Continuous at all x and t	A rapid change would mean that the derivative of the function was very large (either a very large positive or negative number). In the limit of a step function, this would imply an infinite derivative.
First derivative must be continuous at all x and t	A discontinuous first derivative would imply an infinite second derivative, and since the energy of the system is found using the second derivative, a discontinuous first derivative would imply an infinite energy, which again is not physically realistic.

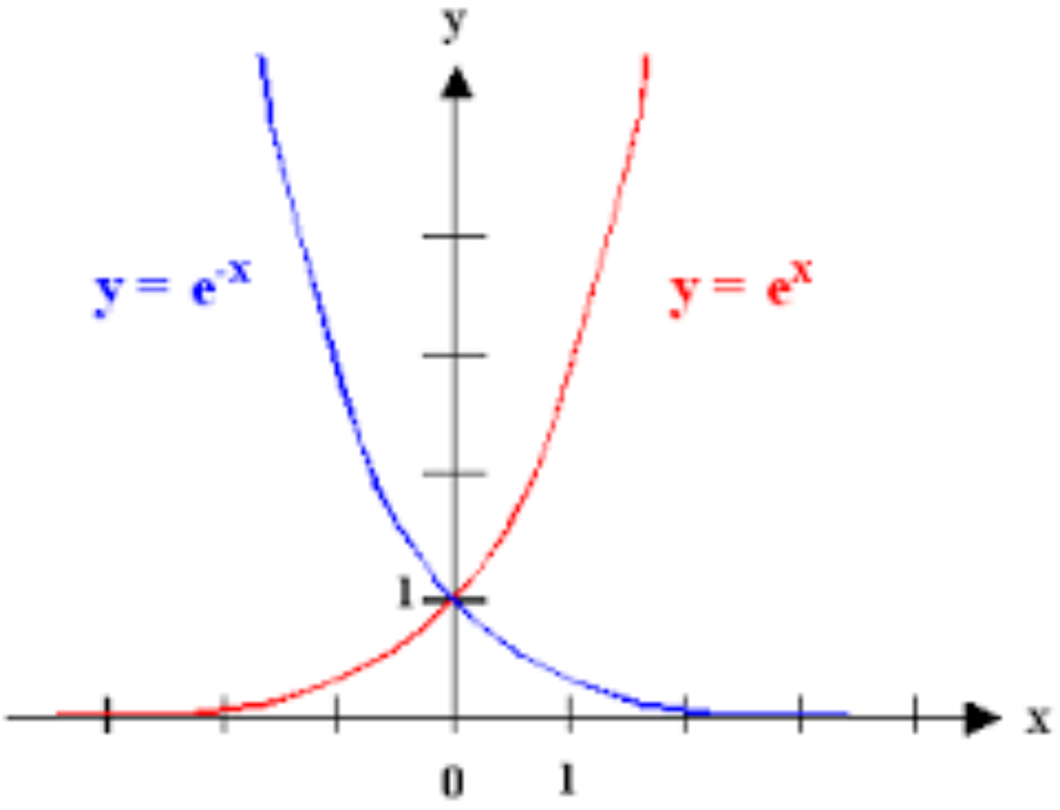
Acceptable or not acceptable form of Ψ

$$(i)\, e^{-x}\,(0,\infty)$$

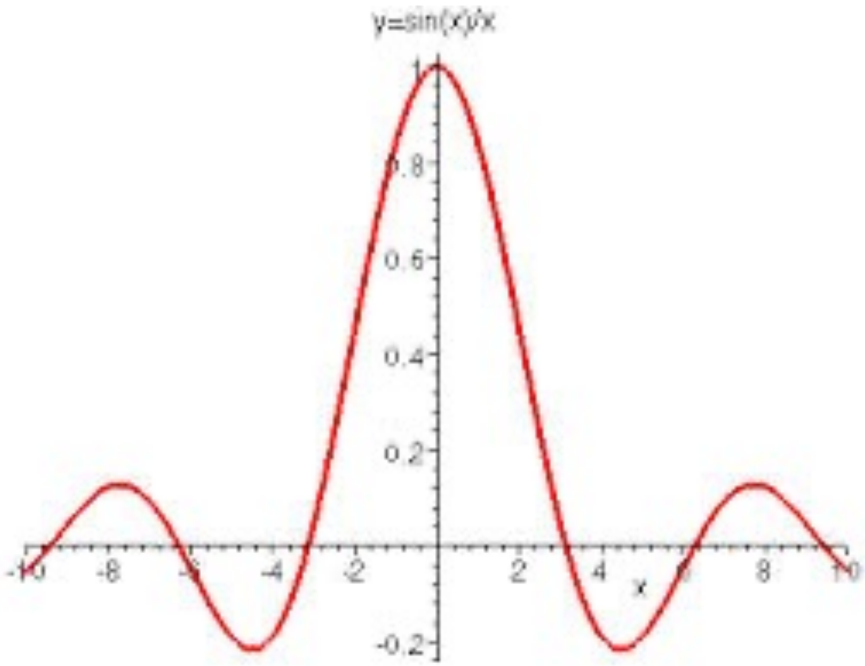
$$(ii)\, e^{-x}\,(-\infty,\infty)$$

$$(iii)\, \frac{\sin x}{x}$$

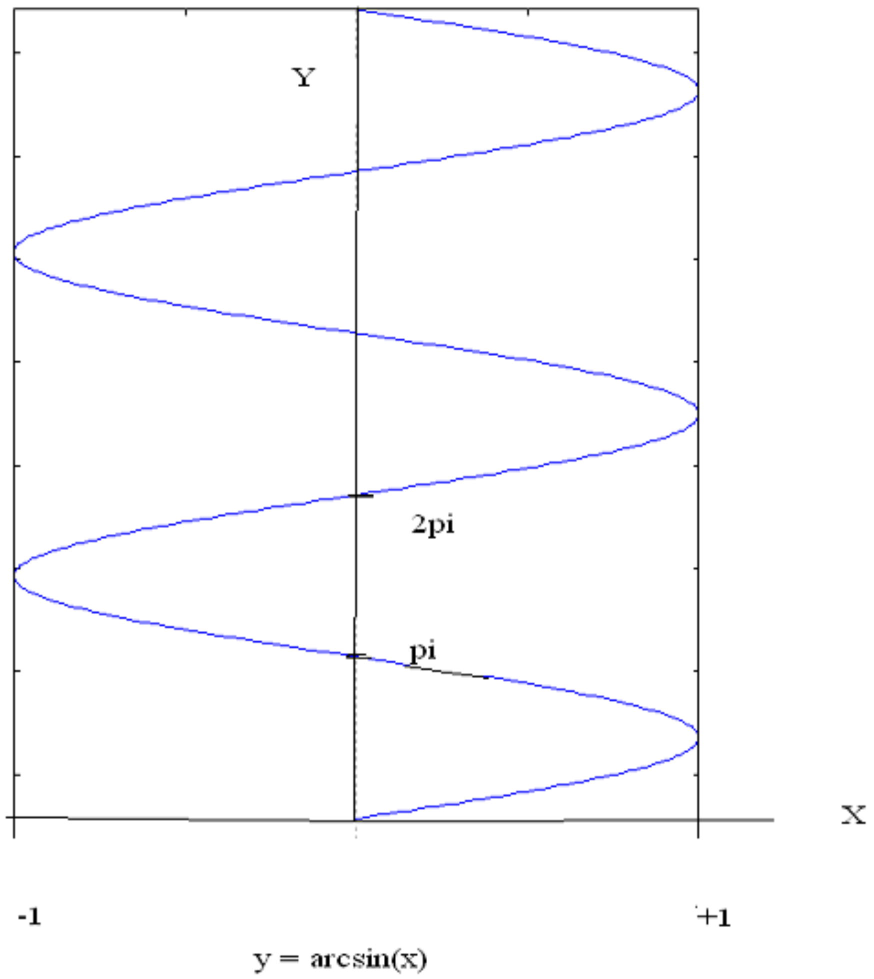
$$(iv)\, \sin^{-1} x$$



Sinx/x



$Sin^{-1}x$



Normalization

Total probability of finding a particle anywhere must be 1: $$\int_{-\infty}^{\infty} P(x)dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

1. This requirement is known as the *Normalization condition*.
2. This condition arises because the Schrodinger Equation is linear in Ψ.
   If Ψ is a solution of Schrodinger equation then so is $c\Psi$ where c is a constant.

Hence if original unnormalized wavefunction is $\Psi(x,t)$, then the normalization integral is:

$$N^2 = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx$$

And the (re-scaled) normalized wavefunction $\Psi_{norm} = (1/N)\,\Psi$.

Summary

- Normalization of Wave-function

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

- Born interpretation

$$\boxed{\Psi^*(x,t)\Psi(x,t)dx = |\Psi(x,t)|^2 dx = P(x,t)dx}$$

- Wave function Ψ need to satisfy few properties:

Finite, Single-valued, Continuous

- Uncertainty in locating the exact position of the electron is related to operations carried out on vectors and the representation of this in matrix form. This leads to the concept of Operators.

Recommended Reading

Wave function sections 6.1 and 6.7