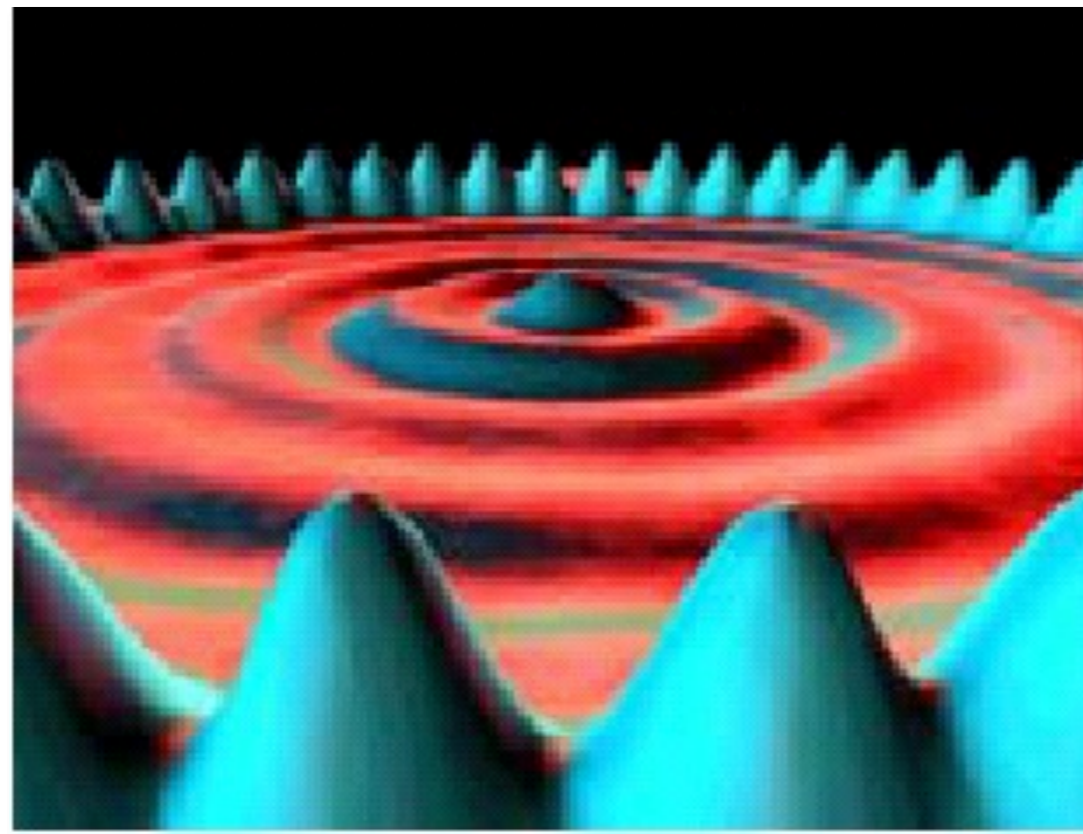
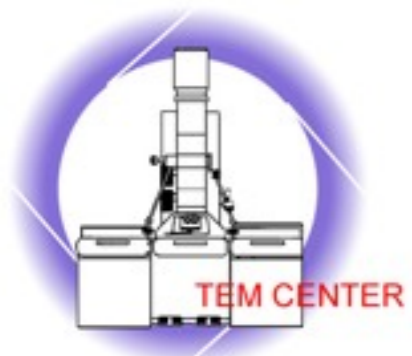


CHAPTER 2

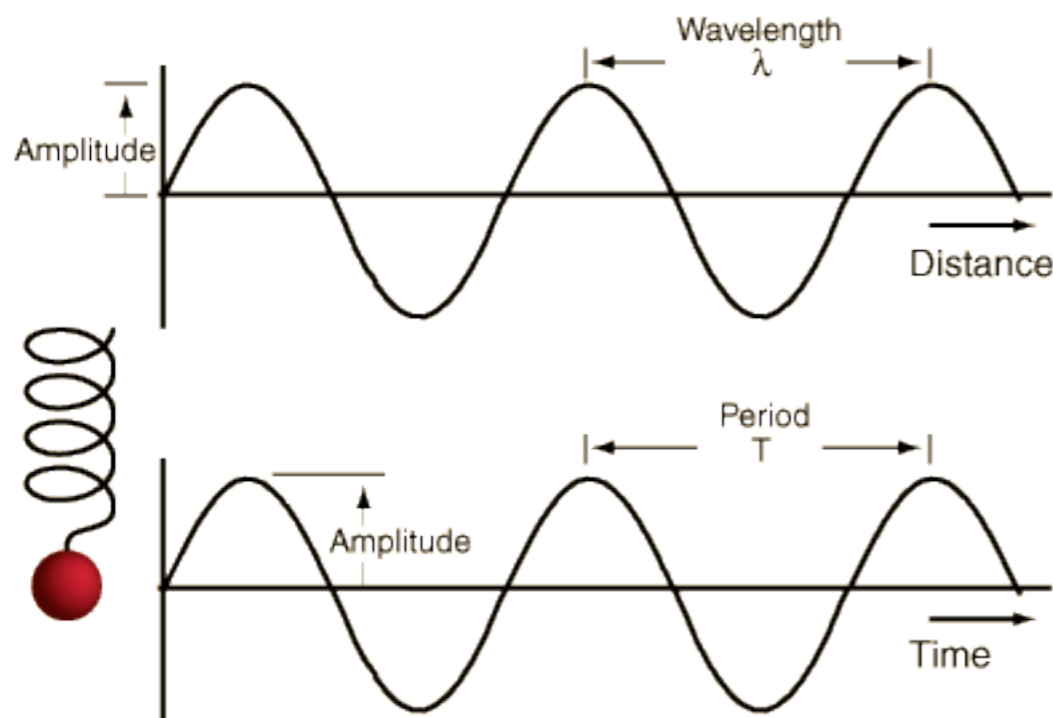
The Wave-Particle Duality





WAVE

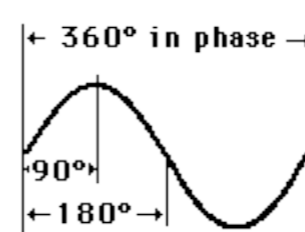
- A **wave** is a disturbance which is periodic in space and time.
- A **vibration** is a disturbance which is periodic in space or time.



$$\psi = A \sin(2\pi x / \lambda - \omega t)$$

$$= A \sin(kx - \omega t)$$

Phase

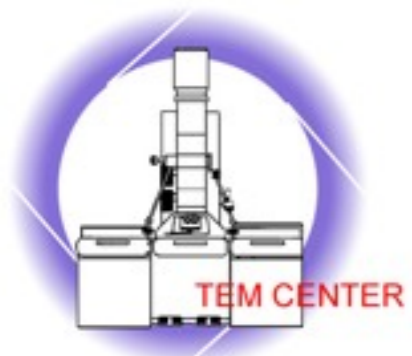


The current I leads the voltage V in phase by angle ϕ . This implies a capacitive circuit.

$$v = \nu \lambda$$

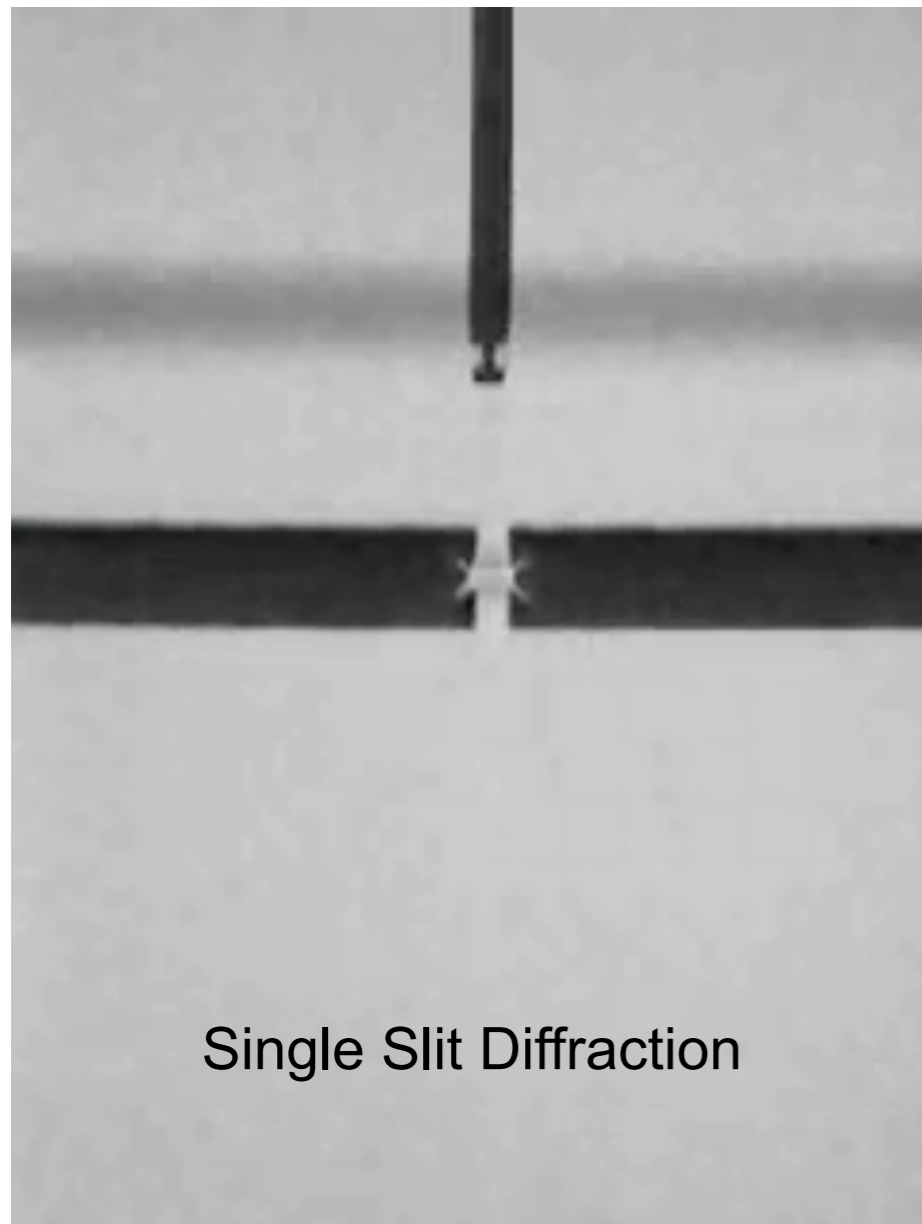
velocity = frequency x wavelength

$$k = \frac{2\pi}{\lambda} \quad \text{wave number}$$

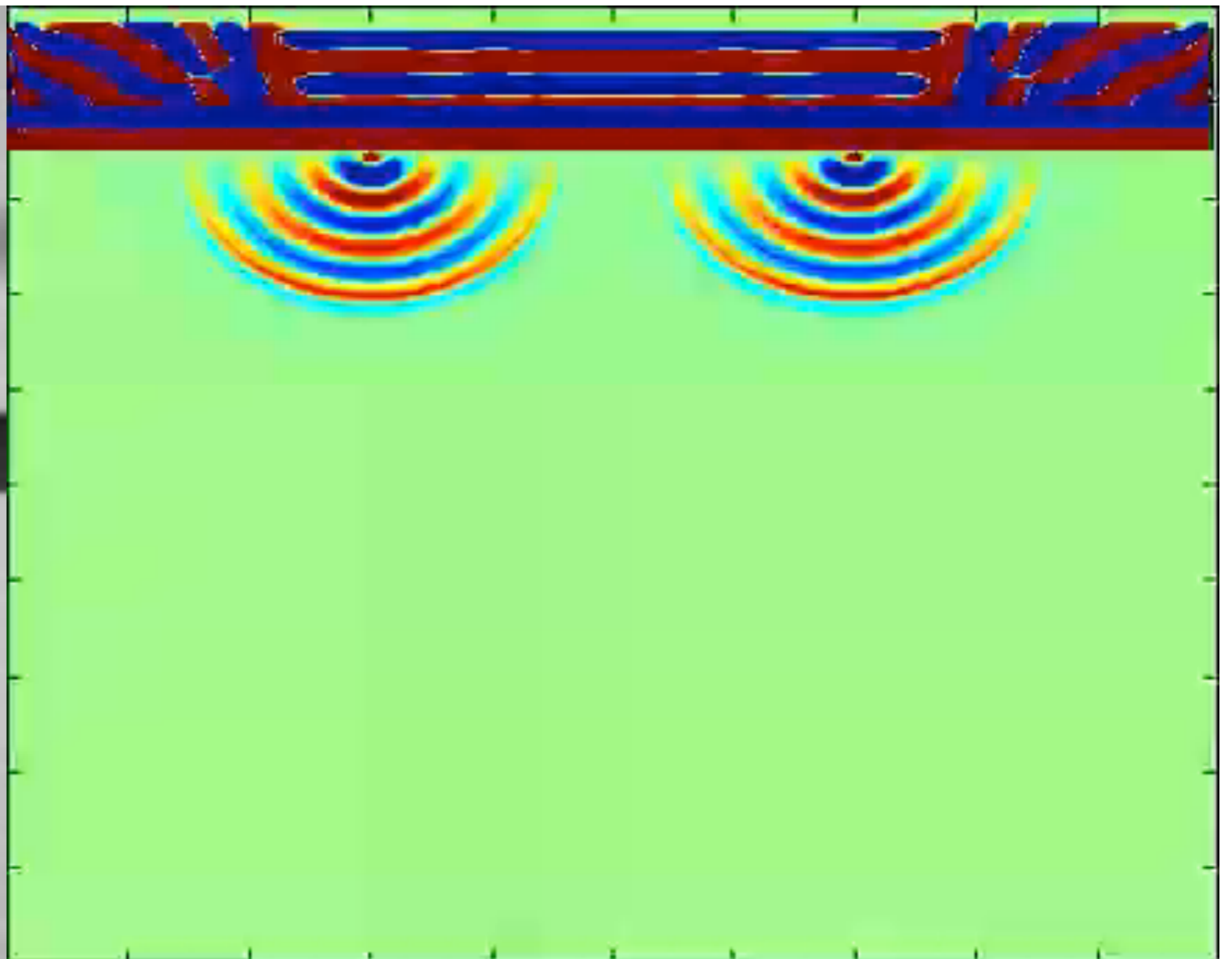


Diffraction

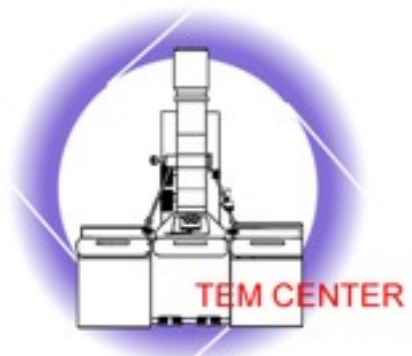
NTHU



single slit

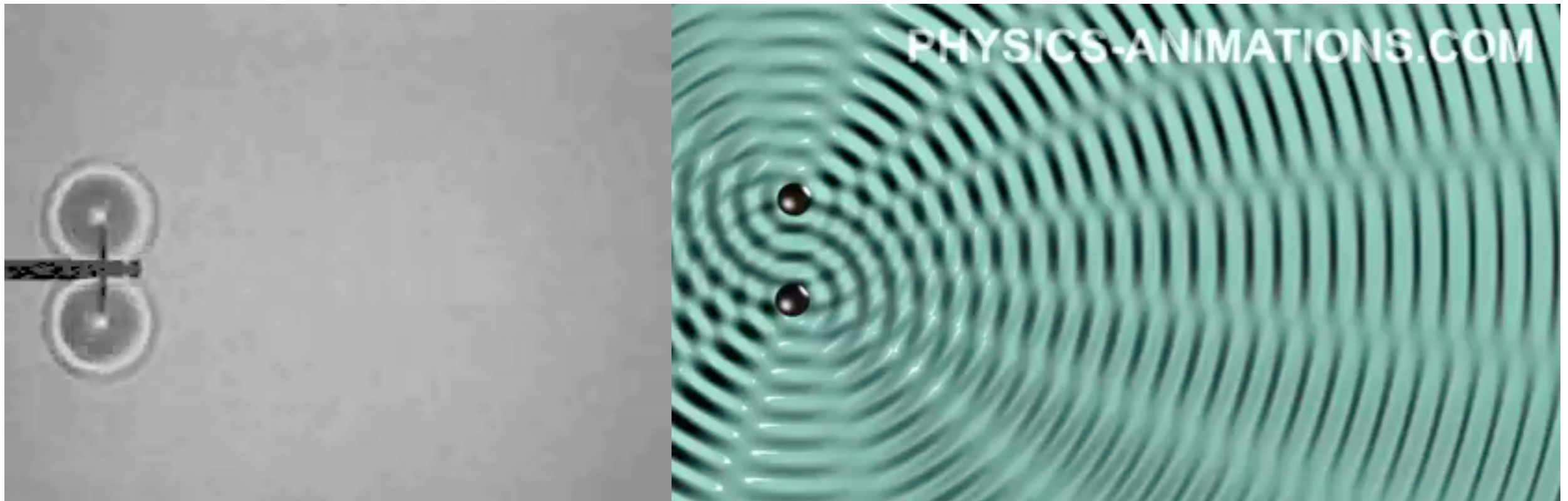


double slit



Interference

NTHU

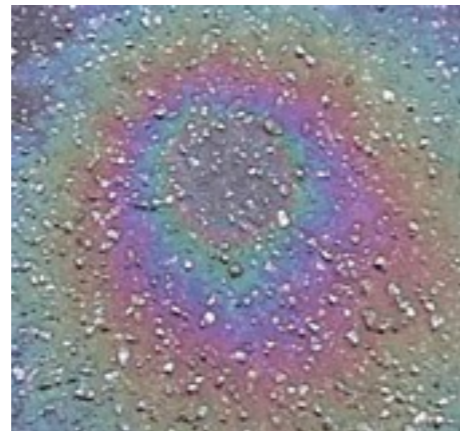




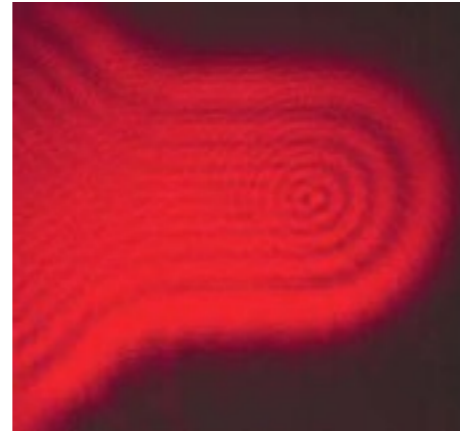
Wave-Particle Duality: Light

NTHU

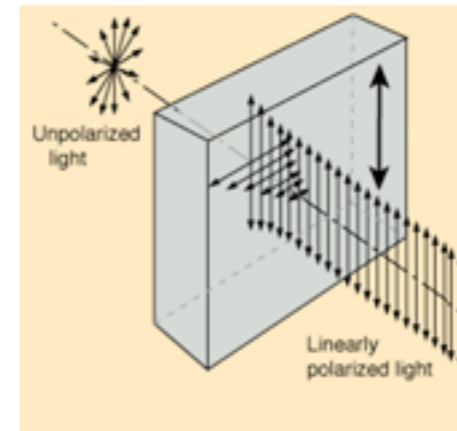
Does light consist of particles or waves? When one focuses upon the different types of phenomena observed with light, a strong case can be built for a wave picture:



Interference



Diffraction



Polarization

By the turn of the 20th century, most physicists were convinced by phenomena like the above that light could be fully described by a wave, with no necessity for invoking a particle nature. But the story was not over.

Phenomenon	Can be explained in terms of waves.	Can be explained in terms of particles.
<u>Reflection</u>		
<u>Refraction</u>		
<u>Interference</u>		
<u>Diffraction</u>		
<u>Polarization</u>		
<u>Photoelectric effect</u>		

Most commonly observed phenomena with light can be explained by waves. But the photoelectric effect suggested a particle nature for light. Then electrons too were found to exhibit dual natures.



Photoelectric Effect

NTHU

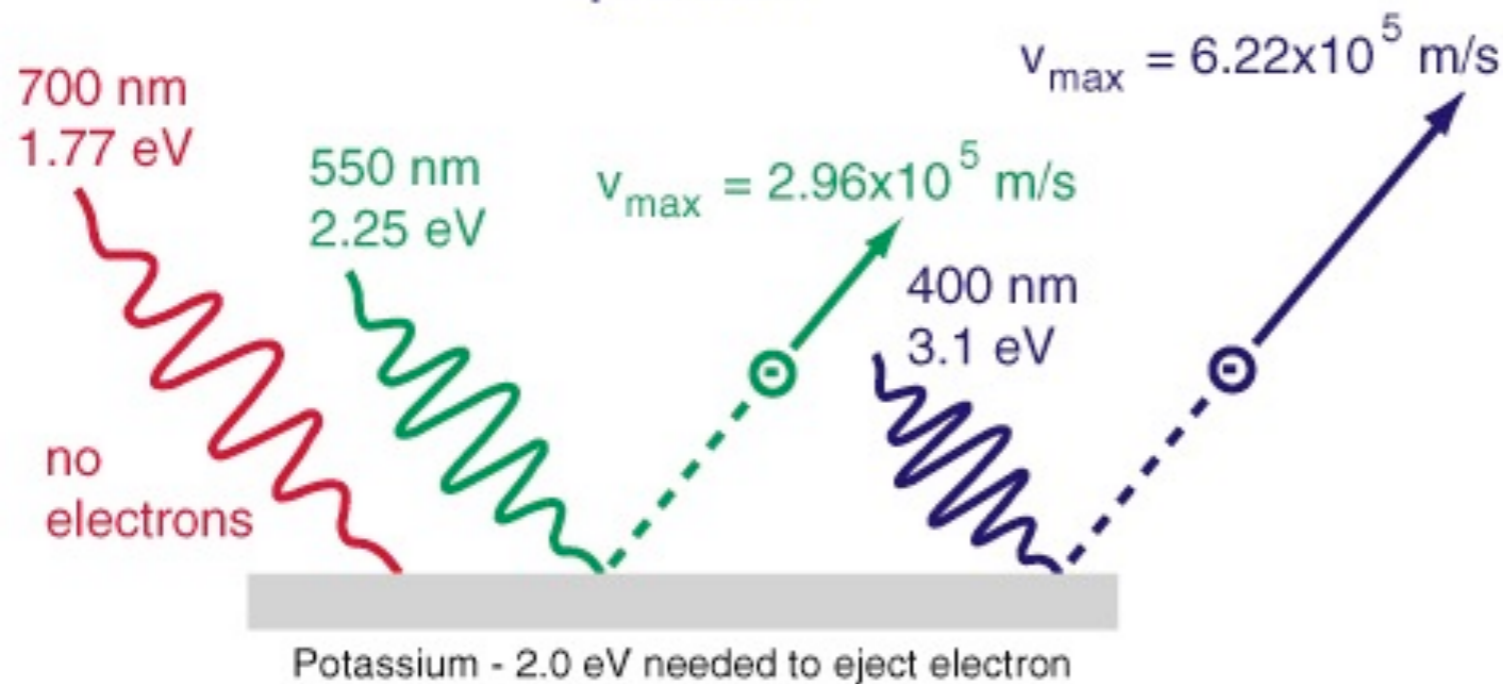
$$E = \nu h = \omega \hbar$$

$$\hbar = \frac{h}{2\pi}$$

$$\omega = 2\pi\nu$$

angle velocity

$$E_{\text{photon}} = h\nu$$



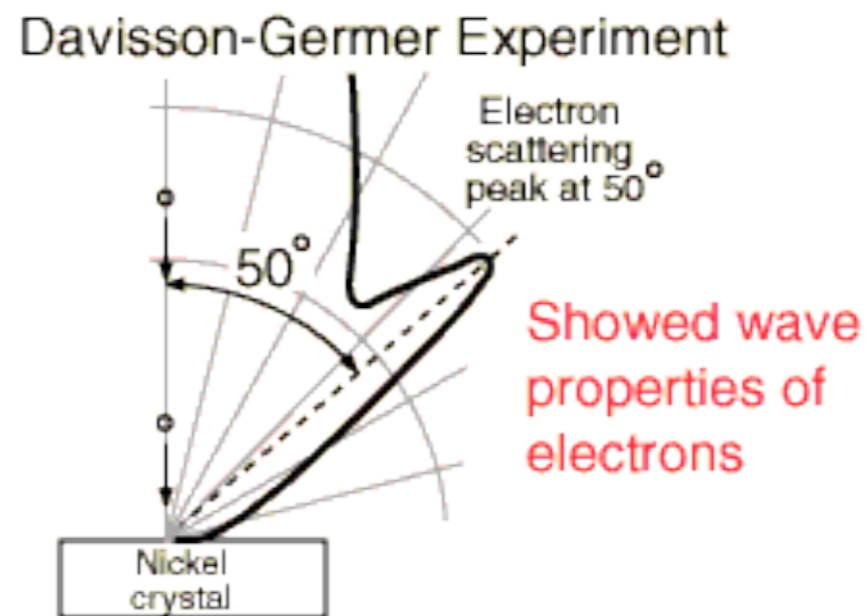
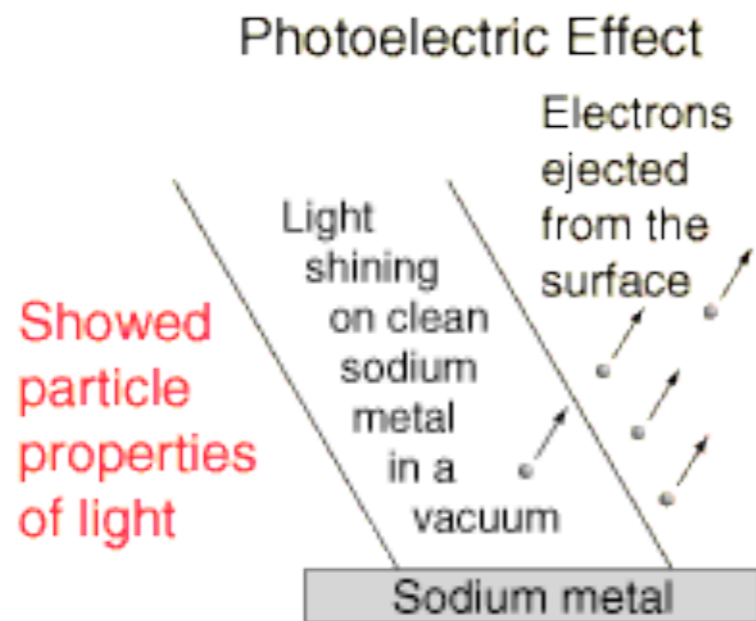
Photoelectric effect

Most commonly observed phenomena with light can be explained by waves. **But the photoelectric effect suggested a particle nature for light.**



Wave-Particle Duality: electron ?

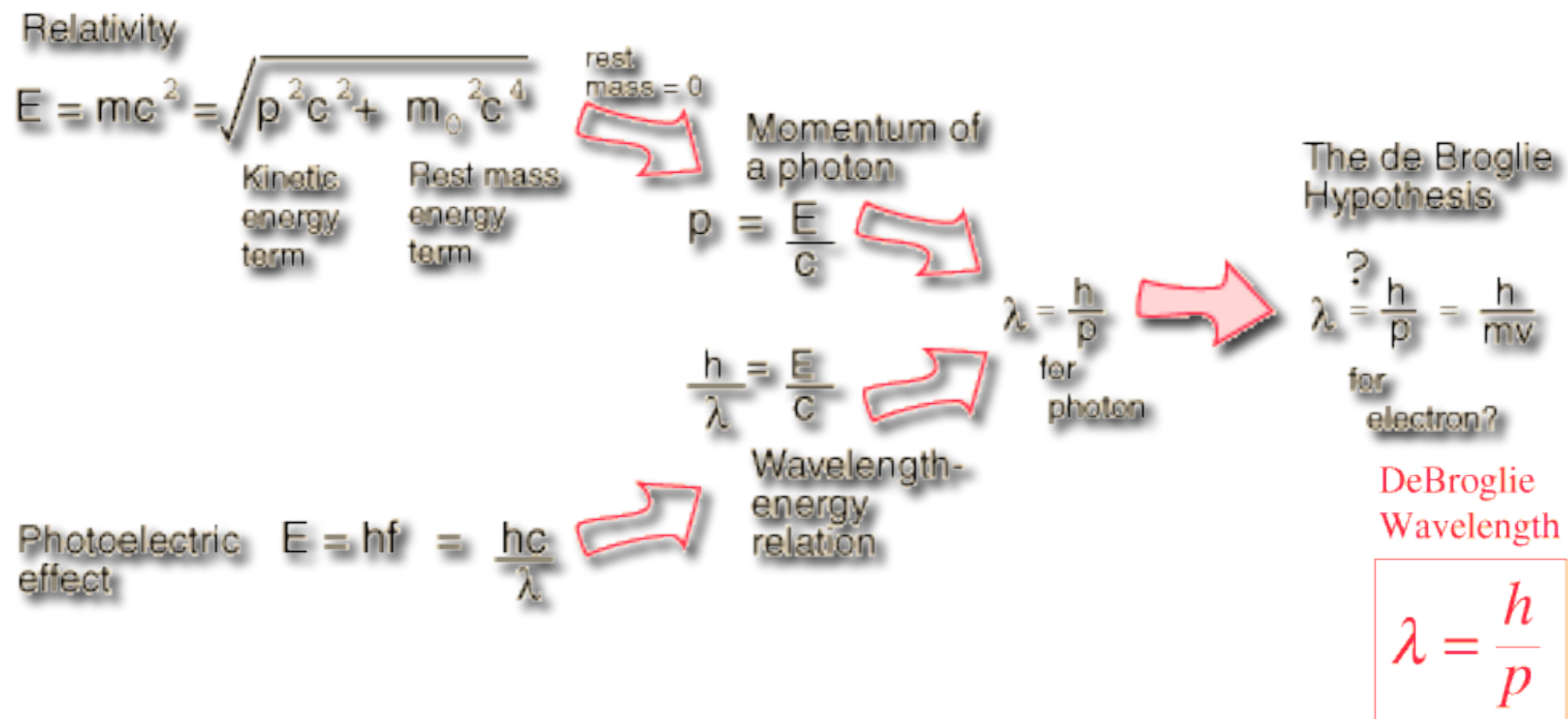
Publicized early in the debate about whether [light](#) was composed of particles or waves, a wave-particle dual nature soon was found to be characteristic of electrons as well. The evidence for the description of light as waves was well established at the turn of the century when the [photoelectric effect](#) introduced firm evidence of a particle nature as well. On the other hand, the particle properties of electrons was well documented when the [DeBroglie hypothesis](#) and the subsequent experiments by [Davisson and Germer](#) established the [wave nature](#) of the electron.





Wave Nature of Electron

As a young student at the University of Paris, Louis DeBroglie had been impacted by [relativity](#) and the [photoelectric effect](#), both of which had been introduced in his lifetime. The photoelectric effect pointed to the particle properties of light, which had been considered to be a wave phenomenon. He wondered if electrons and other "particles" might exhibit wave properties. The application of these two new ideas to light pointed to an interesting possibility:






DeBroglie Wavelengths

DeBroglie
Wavelength

$$\lambda = \frac{h}{p}$$

NTHU

Does this relationship apply to all particles? Consider a pitched baseball:

 \longrightarrow $v = 40 \text{ m/s} = 90 \text{ mi/hr}$
 $m = 0.15 \text{ kg}$

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J s}}{(0.15 \text{ kg})(40 \text{ m/s})} = 1.1 \times 10^{-34} \text{ m}$$

10^{-10} m
Atomic
diameter
 10^{-14} m
Nuclear
Diameter

For an electron accelerated through 100 Volts: $v = 5.9 \times 10^6 \text{ m/s}$

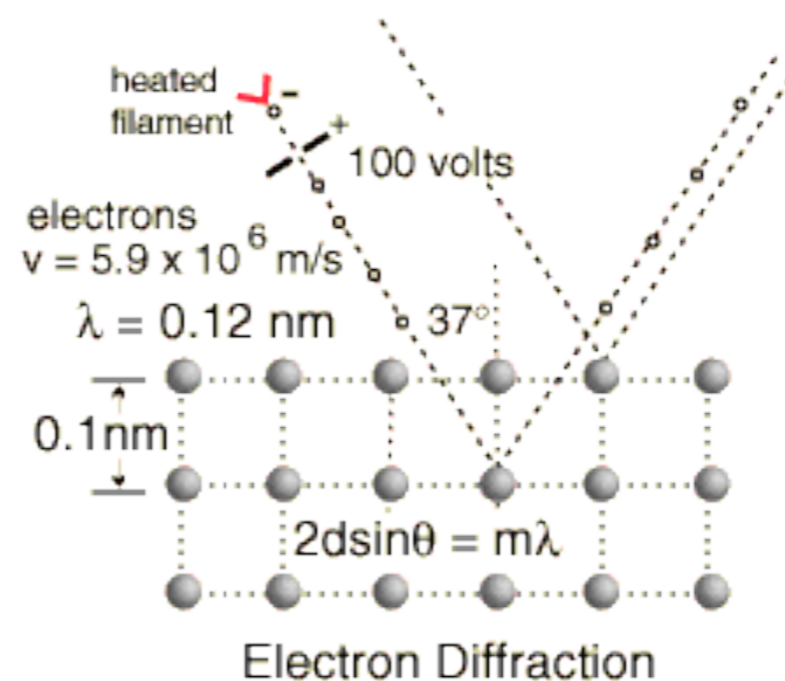
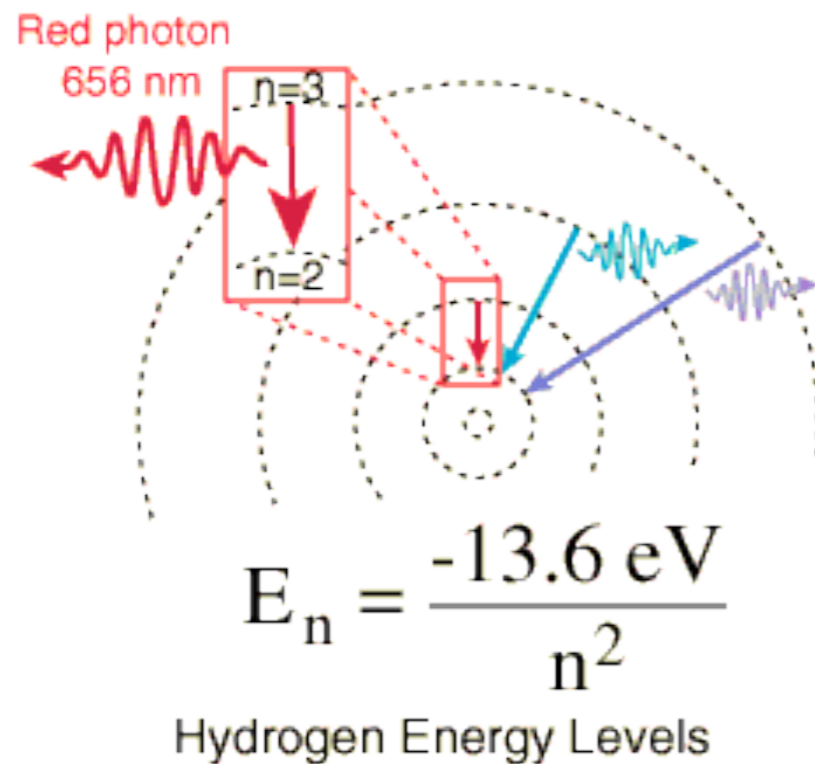
$$\lambda = \frac{6.626 \times 10^{-34} \text{ J s}}{(9.11 \times 10^{-31} \text{ kg})(5.9 \times 10^6 \text{ m/s})} = 1.2 \times 10^{-10} = 0.12 \text{ nm}$$

This is on the order of atomic dimensions and is much shorter than the shortest visible light wavelength of about 390 nm.



Examples of Electron Waves

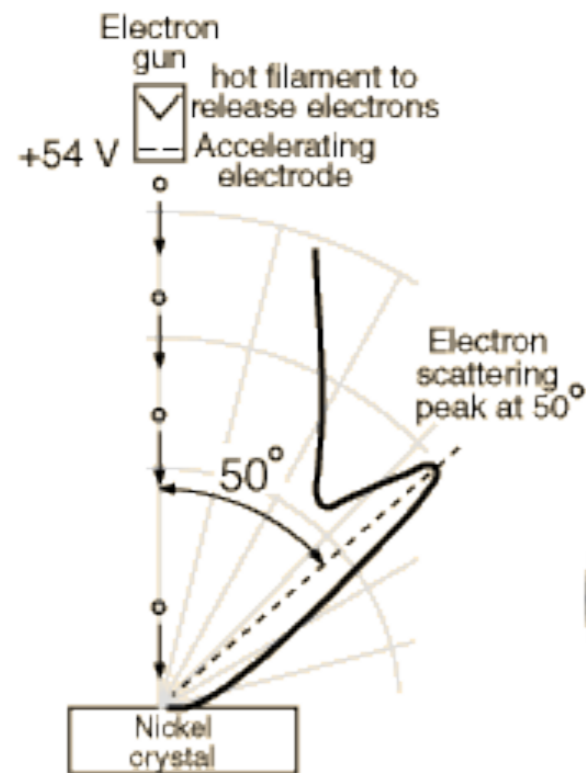
Two specific examples supporting the wave nature of electrons as suggested in the [DeBroglie hypothesis](#) are the discrete atomic energy levels and the diffraction of electrons from crystal planes in solid materials.



The wave nature of the electron must be invoked to explain the behavior of electrons when they are confined to dimensions on the order of the size of an atom. This wave nature is used for the quantum mechanical "[particle in a box](#)" and the result of this calculation is used to describe the density of energy states for [electrons in solids](#).



Davisson-Germer Experiment



Theory

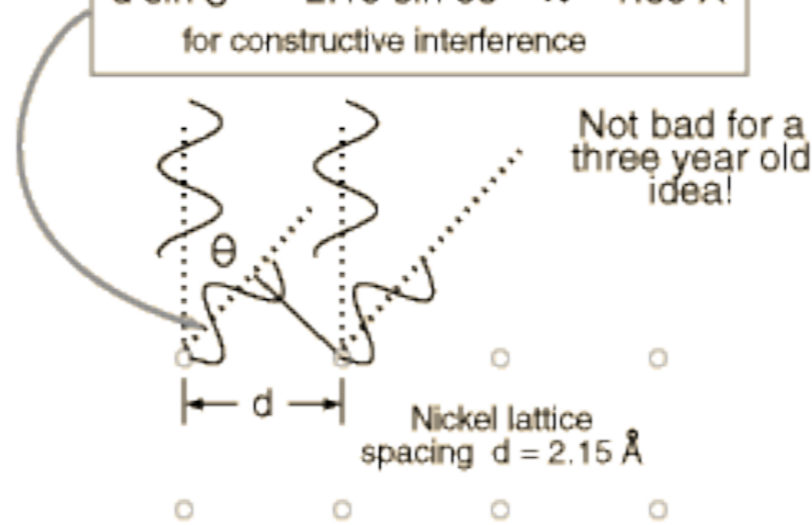
$$\lambda = \frac{h}{mv} = 1.67 \text{ \AA} \text{ for } 54 \text{ V}$$

Experiment

Pathlength difference

$$d \sin \theta = 2.15 \sin 50^\circ = \lambda = 1.65 \text{ \AA}$$

for constructive interference



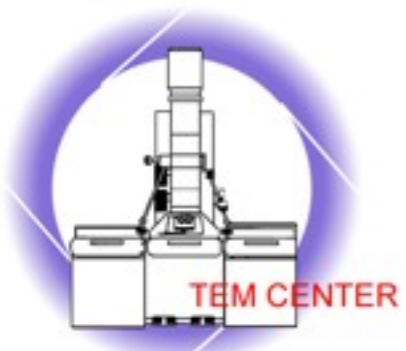
$$\frac{1}{\lambda} = \frac{n}{2d \sin \theta} = \frac{p}{h} = \frac{\sqrt{2mE}}{h} = \frac{\sqrt{2meV}}{h}$$

Electron wavelength *Bragg law* *deBroglie relationship* *Acceleration through voltage V*

λ (nm)	V(keV)
0.0037	100
0.0025	200
0.00197	300
0.00169	400

1924 de Broglie's hypothesis 1927 Davisson-Germer experiment 1929 Nobel Prize for de Broglie

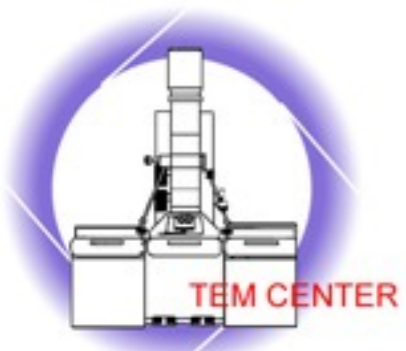
This experiment demonstrated the wave nature of the electron, confirming the earlier hypothesis of deBroglie. Putting wave-particle duality on a firm experimental footing, it represented a major step forward in the development of quantum mechanics. The [Bragg law](#) for diffraction had been applied to x-ray diffraction, but this was the first application to particle waves.



Wave vs. Particle

NTHU

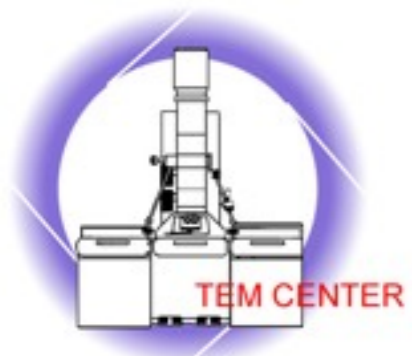




Wave vs. Particle

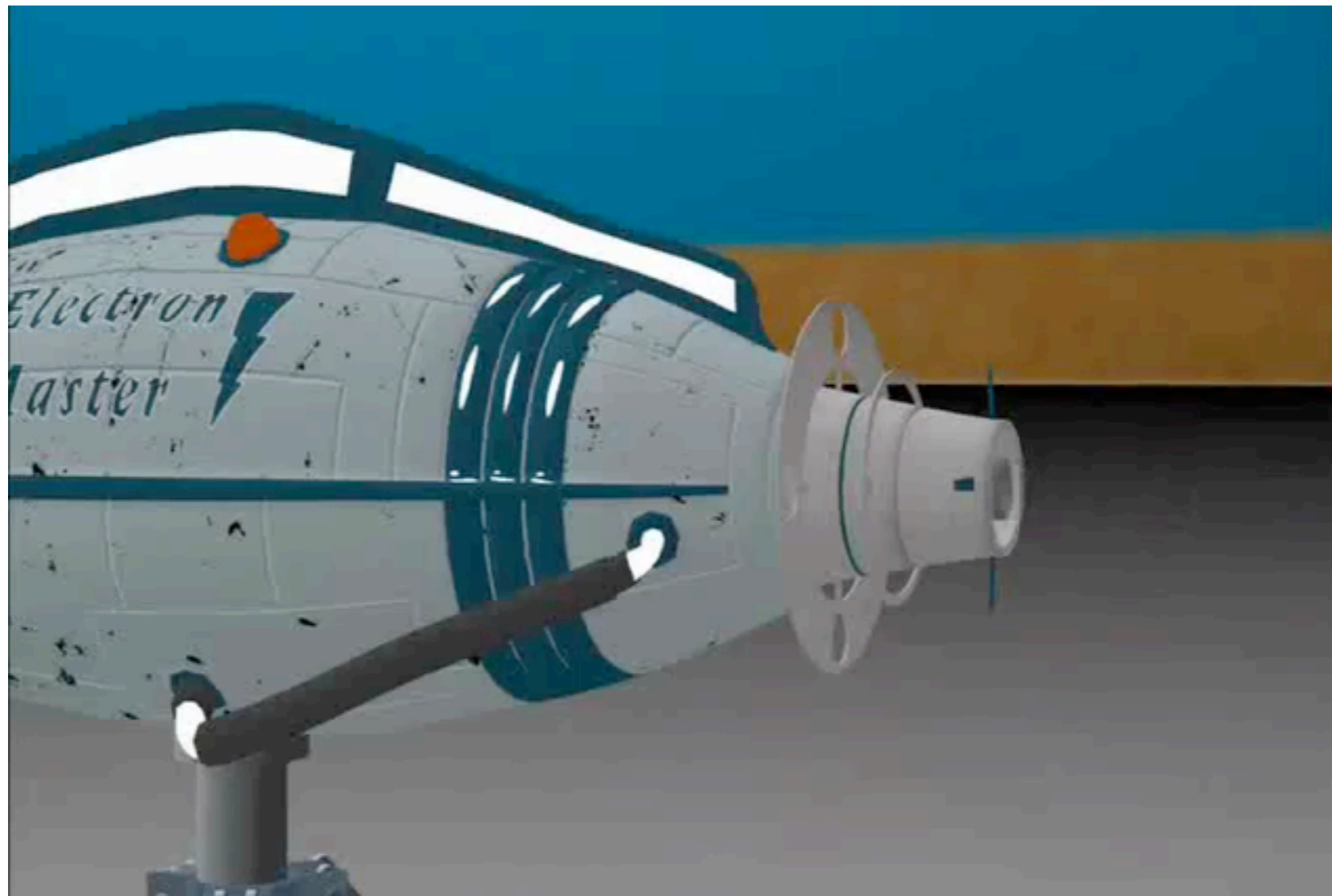
NTHU





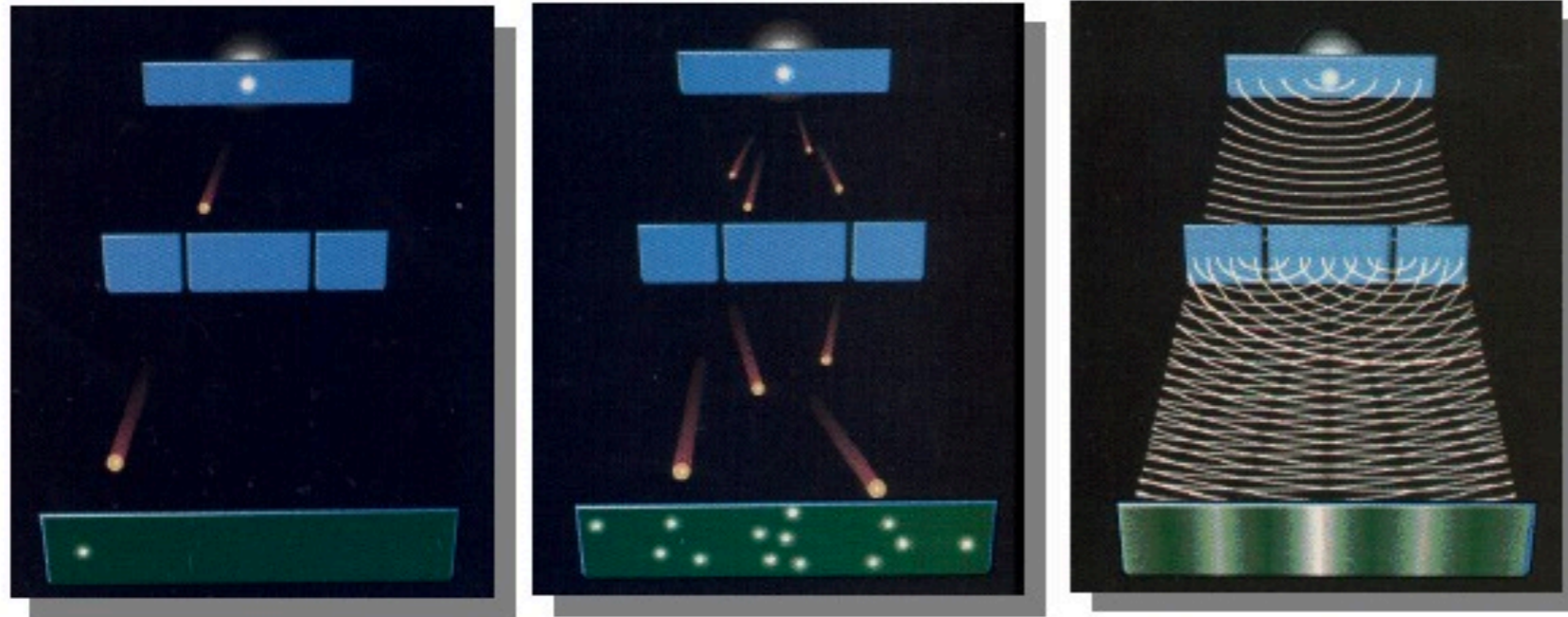
A single electron is a particle wave

NTHU

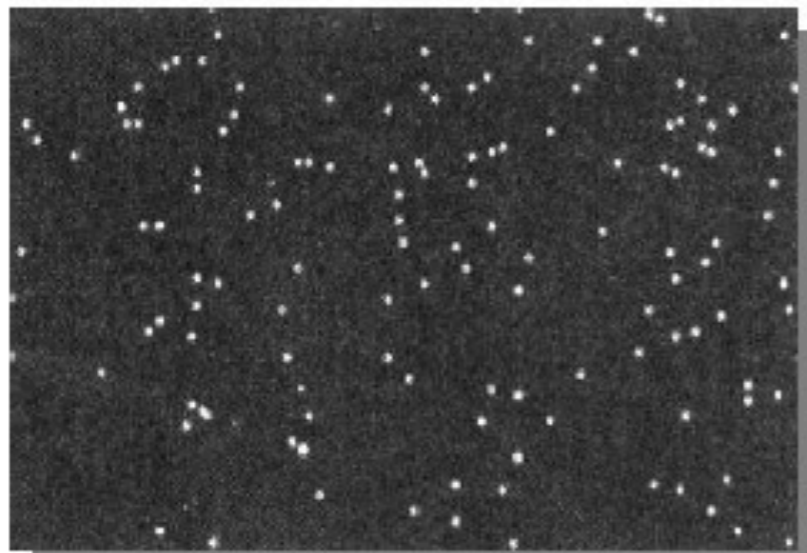


單電子發射的雙狹縫干涉實驗

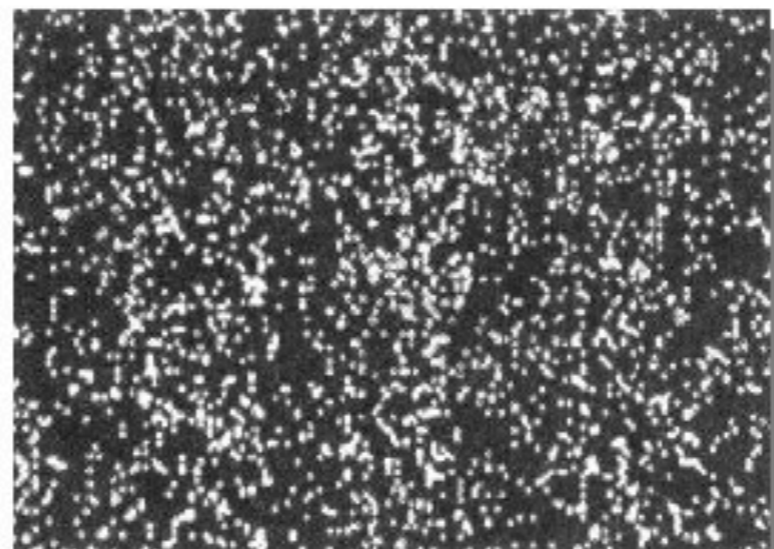
(double-slit experiment with series of single electron emissions)



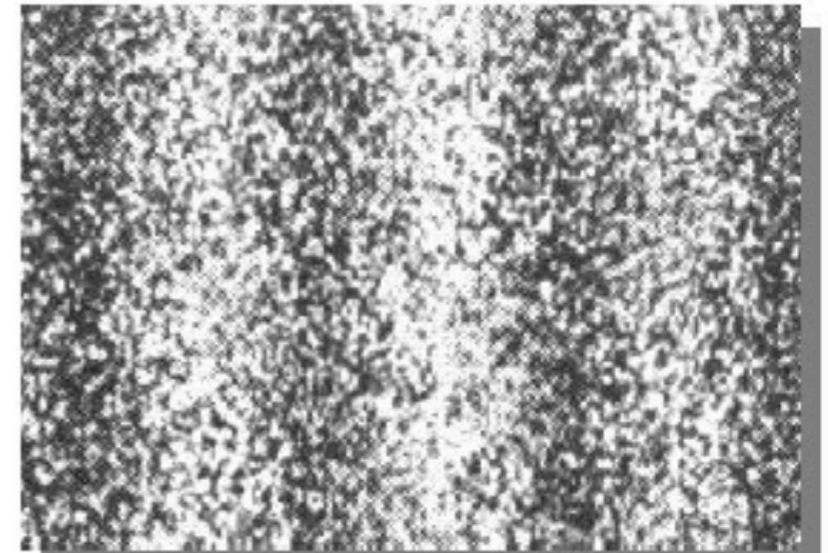
上帝的確是在玩擲骰子的遊戲！



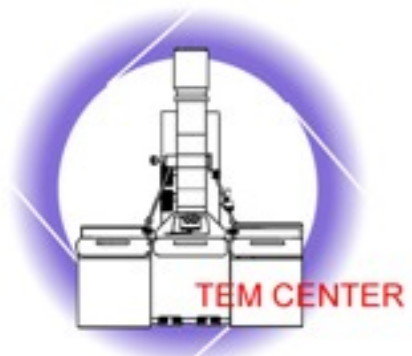
100 electrons



3000 electrons



70,000 electrons

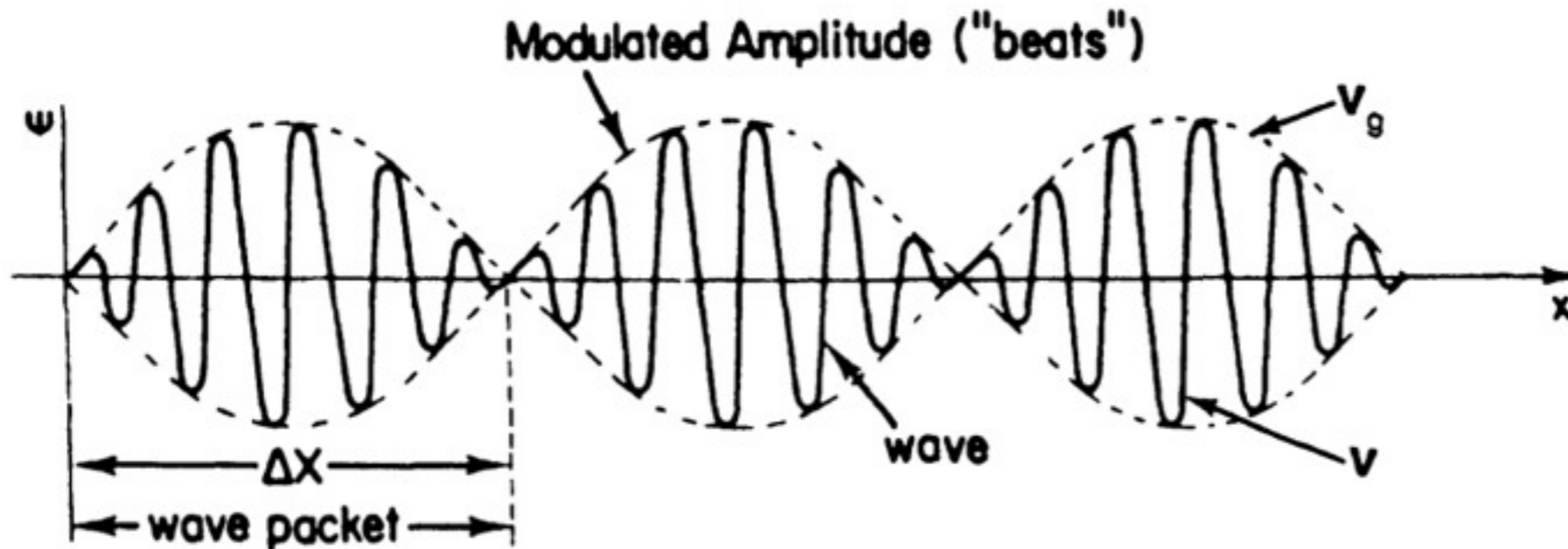


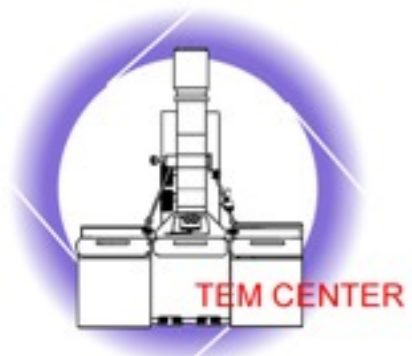
Wave Packet

$$\Psi_1 = \sin[kx - \omega t]$$

$$\Psi_2 = \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

$$\Psi_1 + \Psi_2 = \Psi = \underbrace{2 \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{\text{Modulated amplitude}} \cdot \underbrace{\sin\left[\left(k + \frac{\Delta k}{2}\right)x - \left(\omega + \frac{\Delta\omega}{2}\right)t\right]}_{\text{Sine wave}}$$





Wave Packet

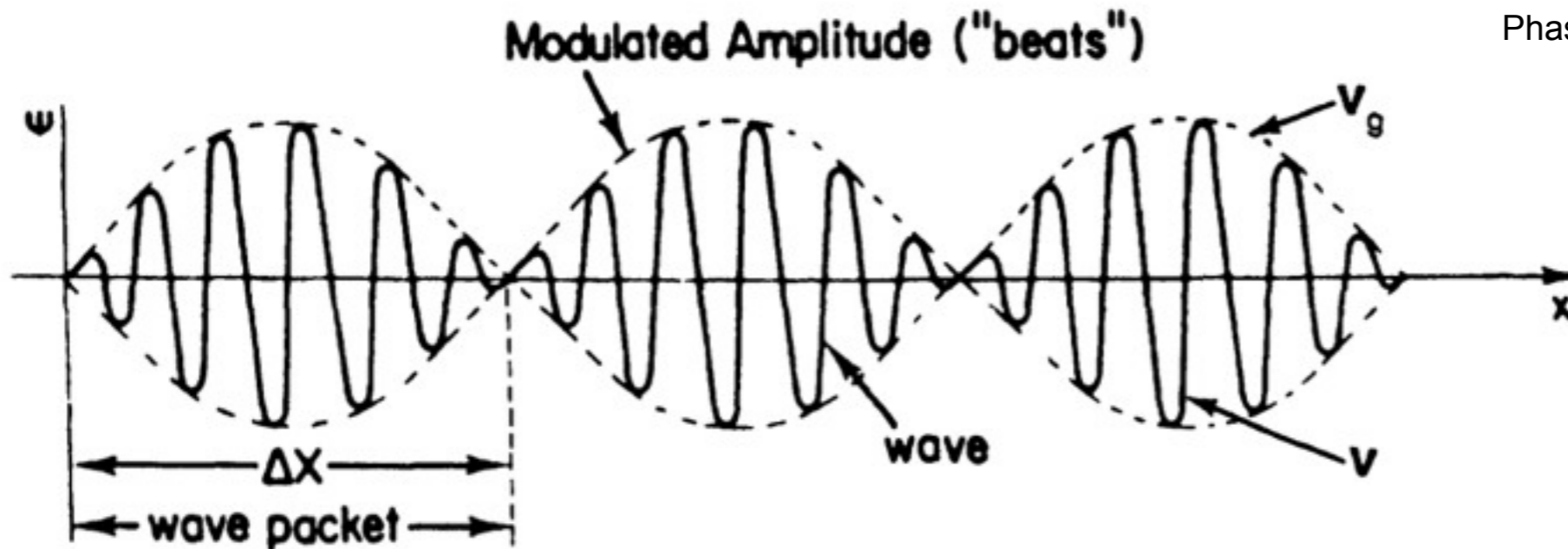
$$\Psi_1 = \sin[kx - \omega t]$$

$$\Psi_2 = \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

$$\Psi_1 + \Psi_2 = \Psi = \underbrace{2 \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{\text{Modulated amplitude}} \cdot \underbrace{\sin\left[\left(k + \frac{\Delta k}{2}\right)x - \left(\omega + \frac{\Delta\omega}{2}\right)t\right]}_{\text{Sine wave}}$$

$$v = \frac{x}{t} = \frac{\omega + \Delta\omega/2}{k + \Delta k/2} = \frac{\omega'}{k'}$$

Phase velocity: velocity of matter wave





Wave Packet

$$\Psi_1 = \sin[kx - \omega t]$$

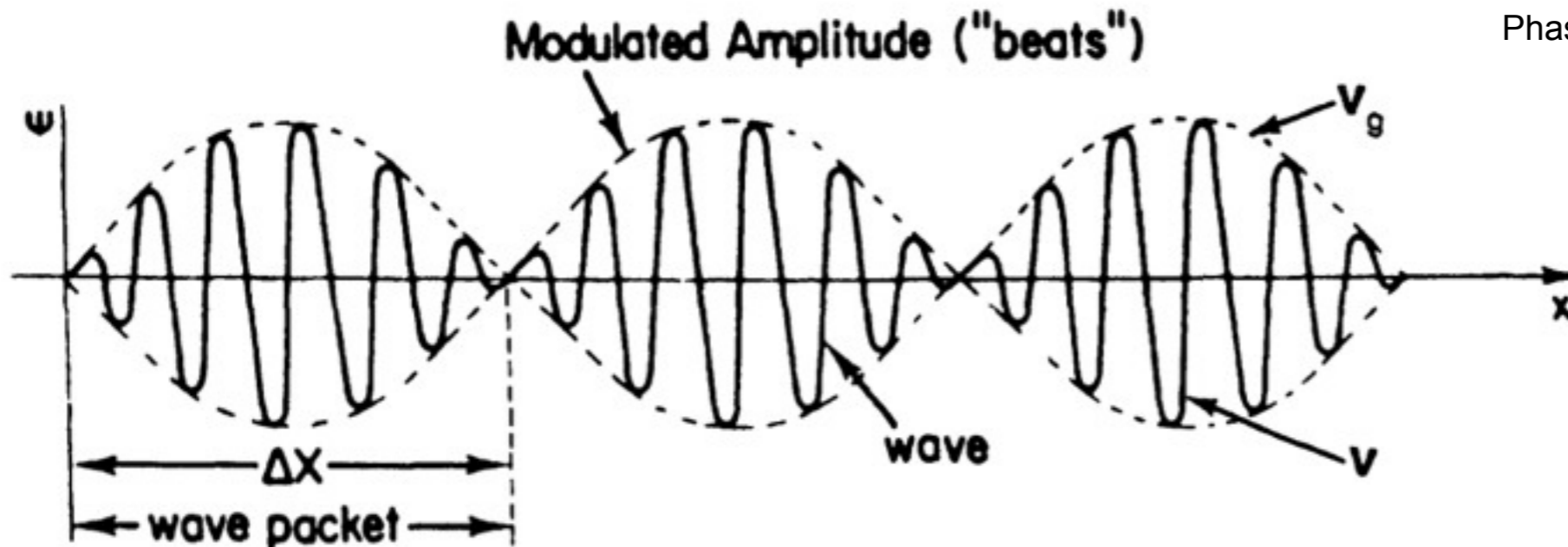
$$\Psi_2 = \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

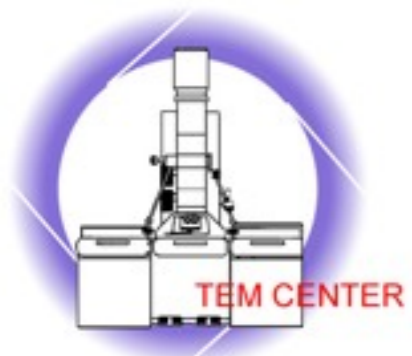
$$\Psi_1 + \Psi_2 = \Psi = \underbrace{2 \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{\text{Modulated amplitude}} \cdot \underbrace{\sin\left[\left(k + \frac{\Delta k}{2}\right)x - \left(\omega + \frac{\Delta\omega}{2}\right)t\right]}_{\text{Sine wave}}$$

$$v = \frac{x}{t} = \frac{\omega + \Delta\omega/2}{k + \Delta k/2} = \frac{\omega'}{k'}$$

Phase velocity: velocity of matter wave

Dispersion





Wave Packet

$$\Psi_1 = \sin[kx - \omega t]$$

$$\Psi_2 = \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

$$\Psi_1 + \Psi_2 = \Psi = \underbrace{2 \cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{\text{Modulated amplitude}} \cdot \underbrace{\sin\left[\left(k + \frac{\Delta k}{2}\right)x - \left(\omega + \frac{\Delta\omega}{2}\right)t\right]}_{\text{Sine wave}}$$

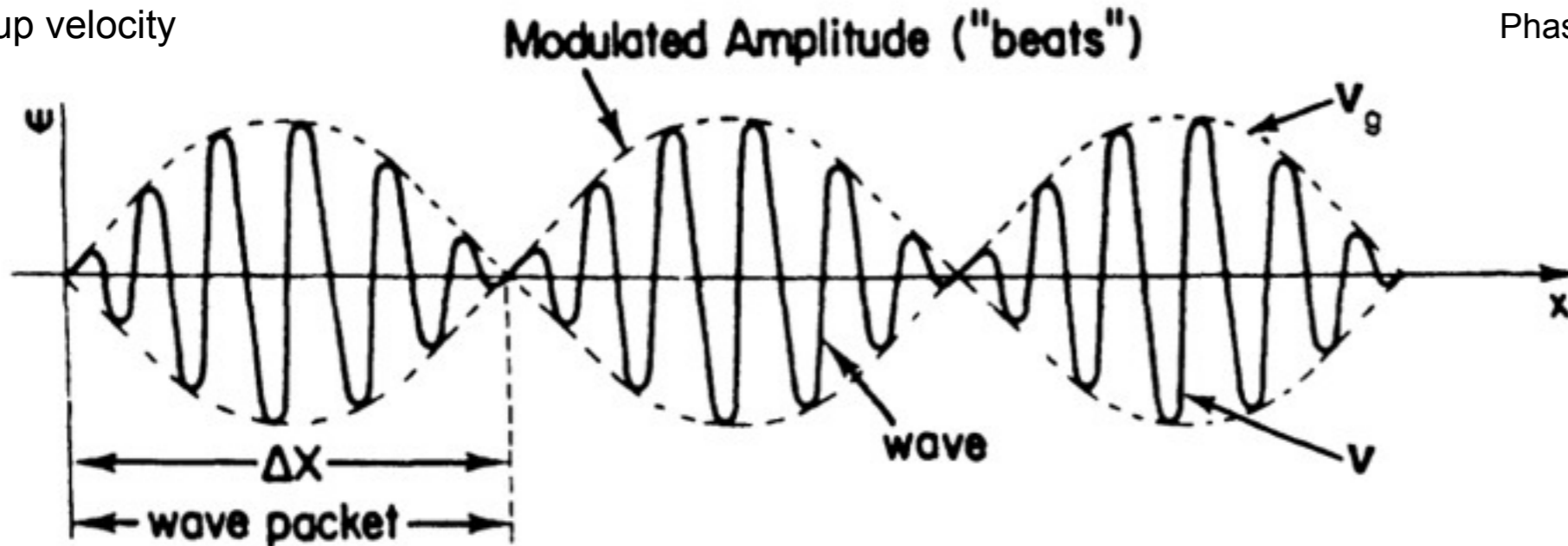
$$v_g = \frac{x}{t} = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$$

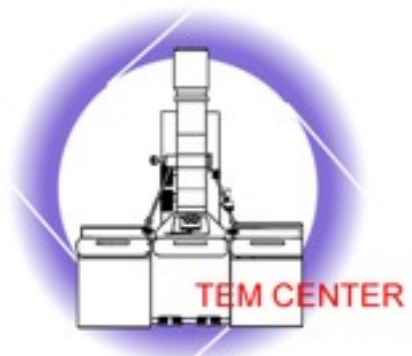
group velocity

$$v = \frac{x}{t} = \frac{\omega + \Delta\omega/2}{k + \Delta k/2} = \frac{\omega'}{k'}$$

Phase velocity: velocity of matter wave

Dispersion



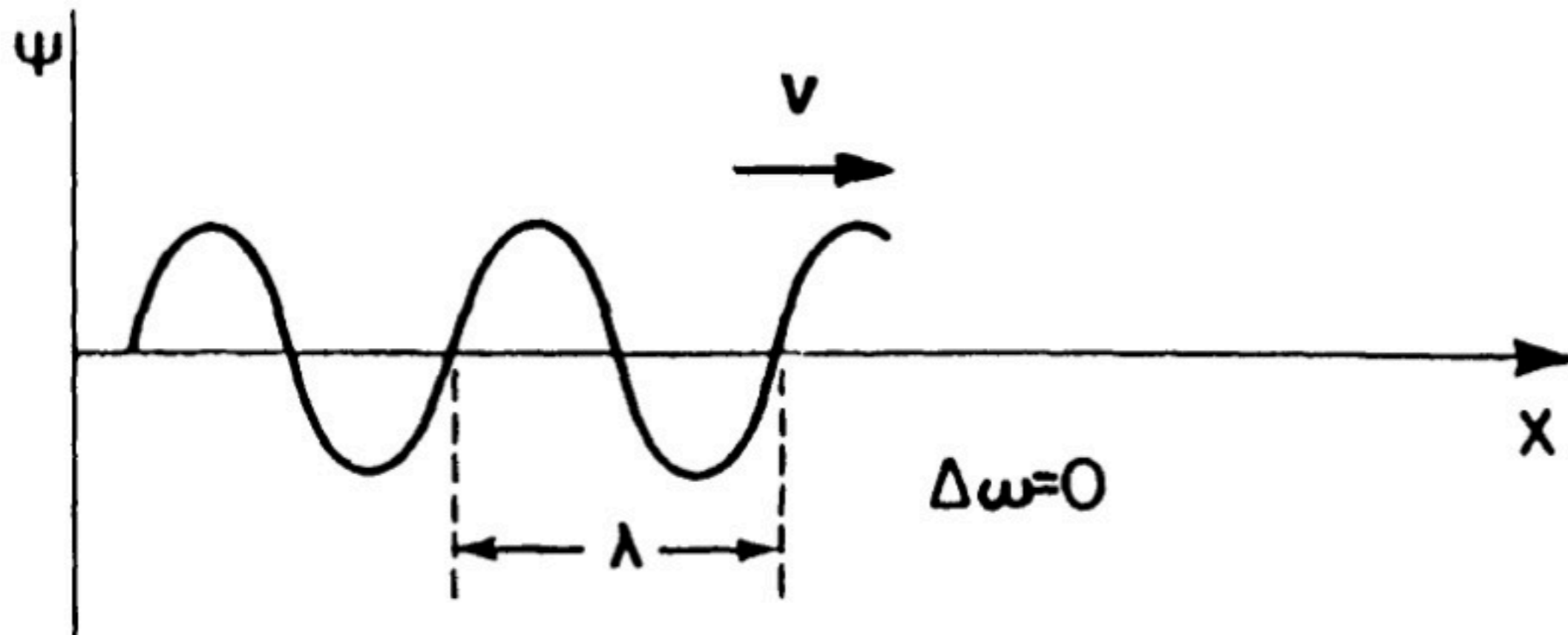


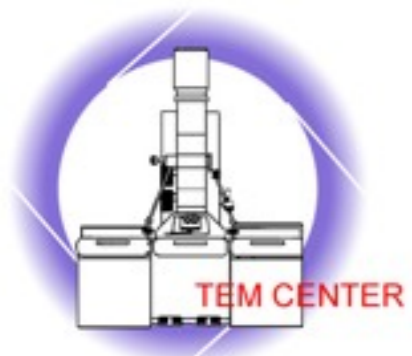
Monochromatic Wave

NTHU

$$\Delta\omega = 0 \text{ and } \Delta k = 0$$

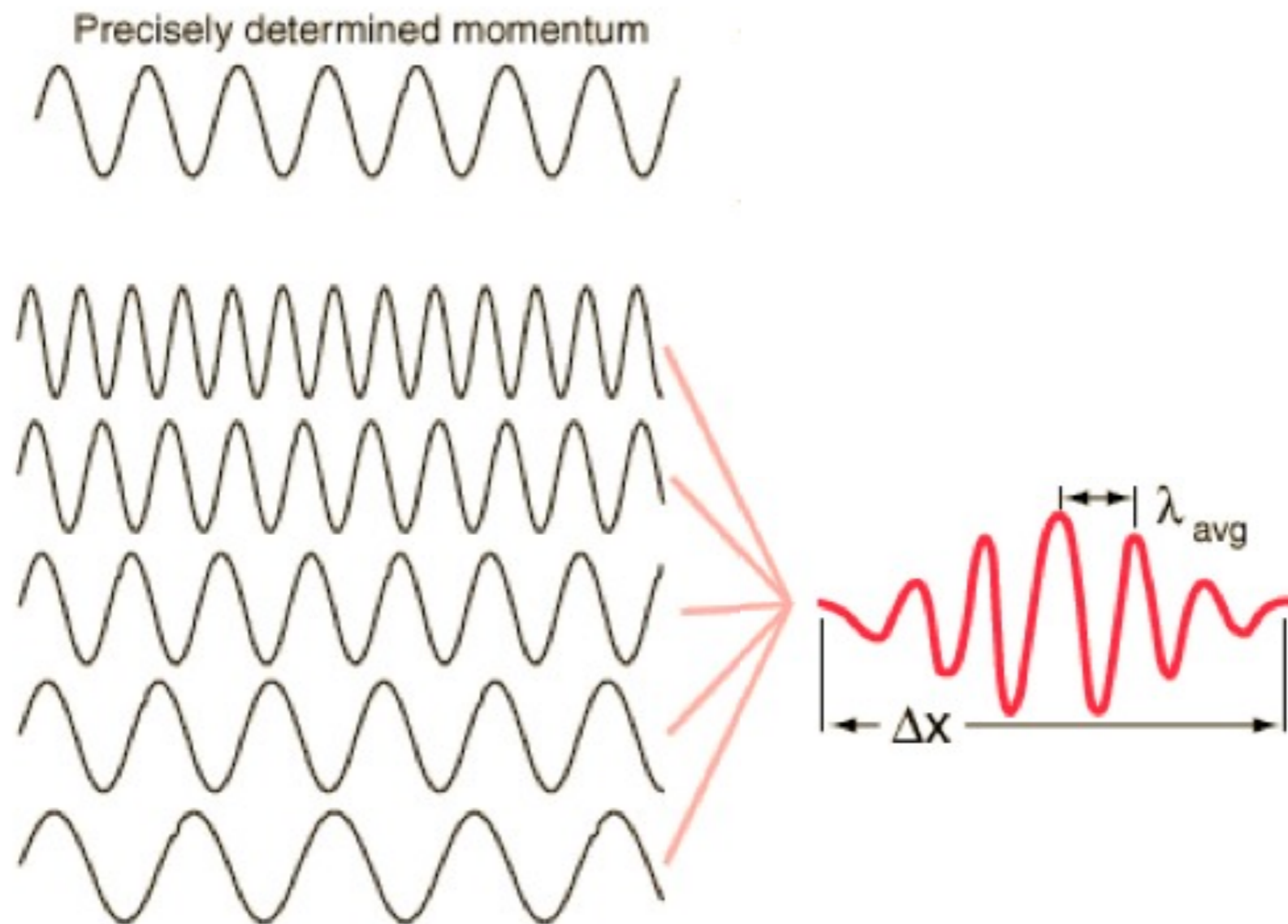
~ infinity length of wave packet





Chromatic Wave

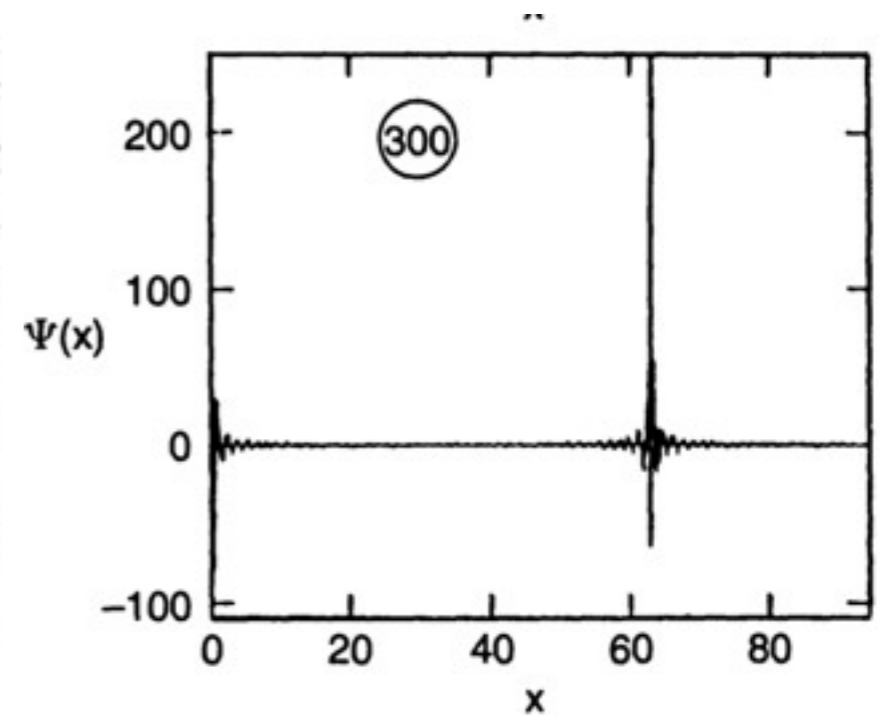
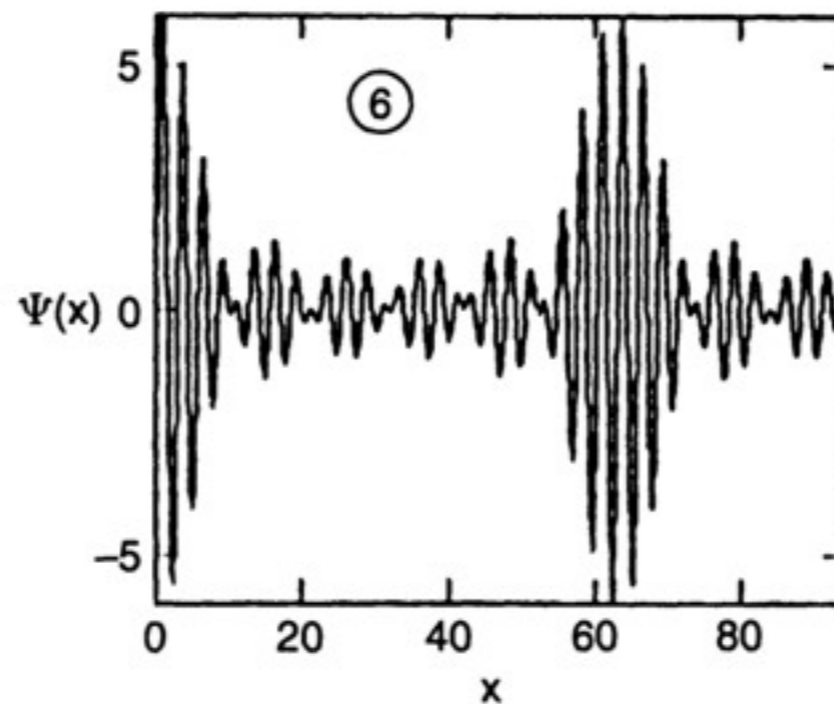
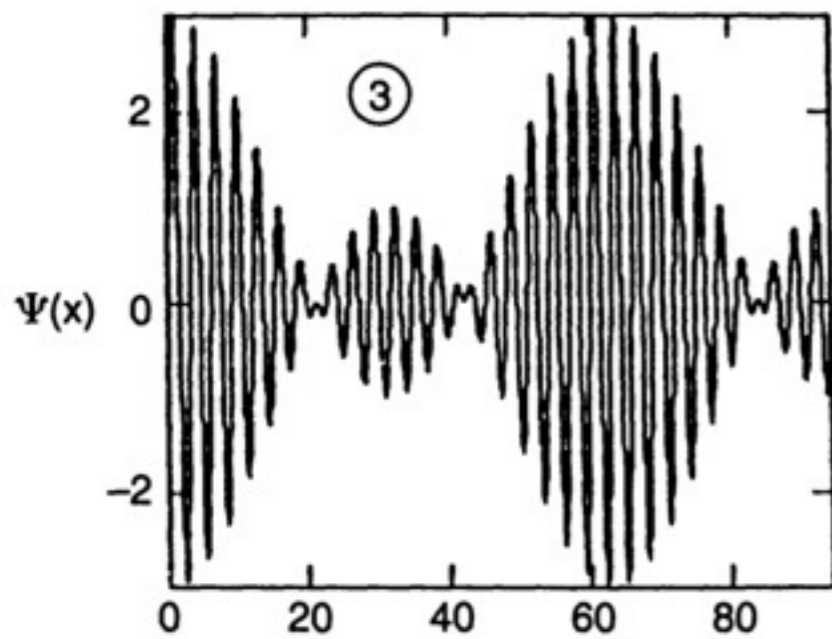
$\Delta\omega$ and Δk could be assumed to be very large





Heisenberg's uncertainty principle

NTHU



The Uncertainty Principle

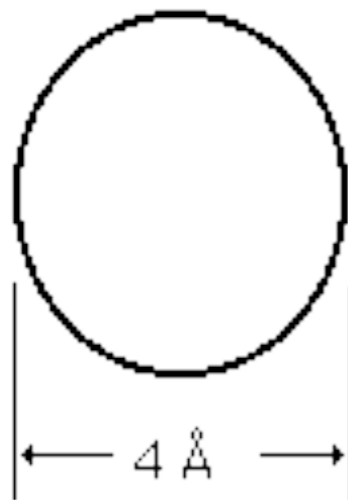
$$\Delta x \Delta p > \frac{\hbar}{2}$$
$$\Delta E \Delta t > \frac{\hbar}{2}$$



Heisenberg's uncertainty principle

NTHU

The **uncertainty principle** contains implications about the energy which would be required to contain a particle within a given volume.



Assume atomic size = 4 Å

Nuclear size = $\frac{1}{20,000} \times 4 \text{ Å}$

Using the atomic size as the uncertainty in position

$$\Delta p = \frac{h}{\Delta x} = 1.66 \times 10^{-24} \text{ kg m/s}$$

Assume $\Delta p = p$

and $E = \frac{p^2}{2m}$

Energy to:

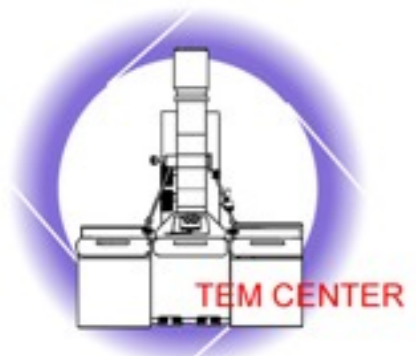
Confine electron in atom: 9.4 eV

Confine proton in nucleus: 2.05 MeV

Confine electron in nucleus: 3.77 GeV

These are in the range of observed atomic and nuclear processes.

This is about a factor of a thousand above the observed energies of nuclear processes, indicating that the electron cannot be confined in the nucleus.



NTHU



Confinement Calculation

Confinement in atom

Assume atomic size = $4 \text{ \AA} = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 1.66 \times 10^{-24} \text{ kg m/s}$$

$$\Delta p = p; E = \frac{p^2}{2m};$$

For electron:

$$E = \frac{(1.66 \times 10^{-24} \text{ kg m/s})^2}{2(9.11 \times 10^{-31} \text{ kg})(1.6 \times 10^{-19} \text{ J/eV})}$$

$$E = 9.4 \text{ eV}$$

Confinement in nucleus

Nuclear size = $\frac{1}{20,000} \times 4 \text{ \AA} = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 3.31 \times 10^{-20} \text{ kg m/s}$$

For electron:

$$E = \frac{(3.31 \times 10^{-20} \text{ kg m/s})^2}{2(9.11 \times 10^{-31} \text{ kg})(1.6 \times 10^{-19} \text{ J/eV})}$$

$$E = 3.77 \times 10^9 \text{ eV} = 3.77 \text{ GeV}$$

For proton, divide by $m_p/m_e = 1836$:

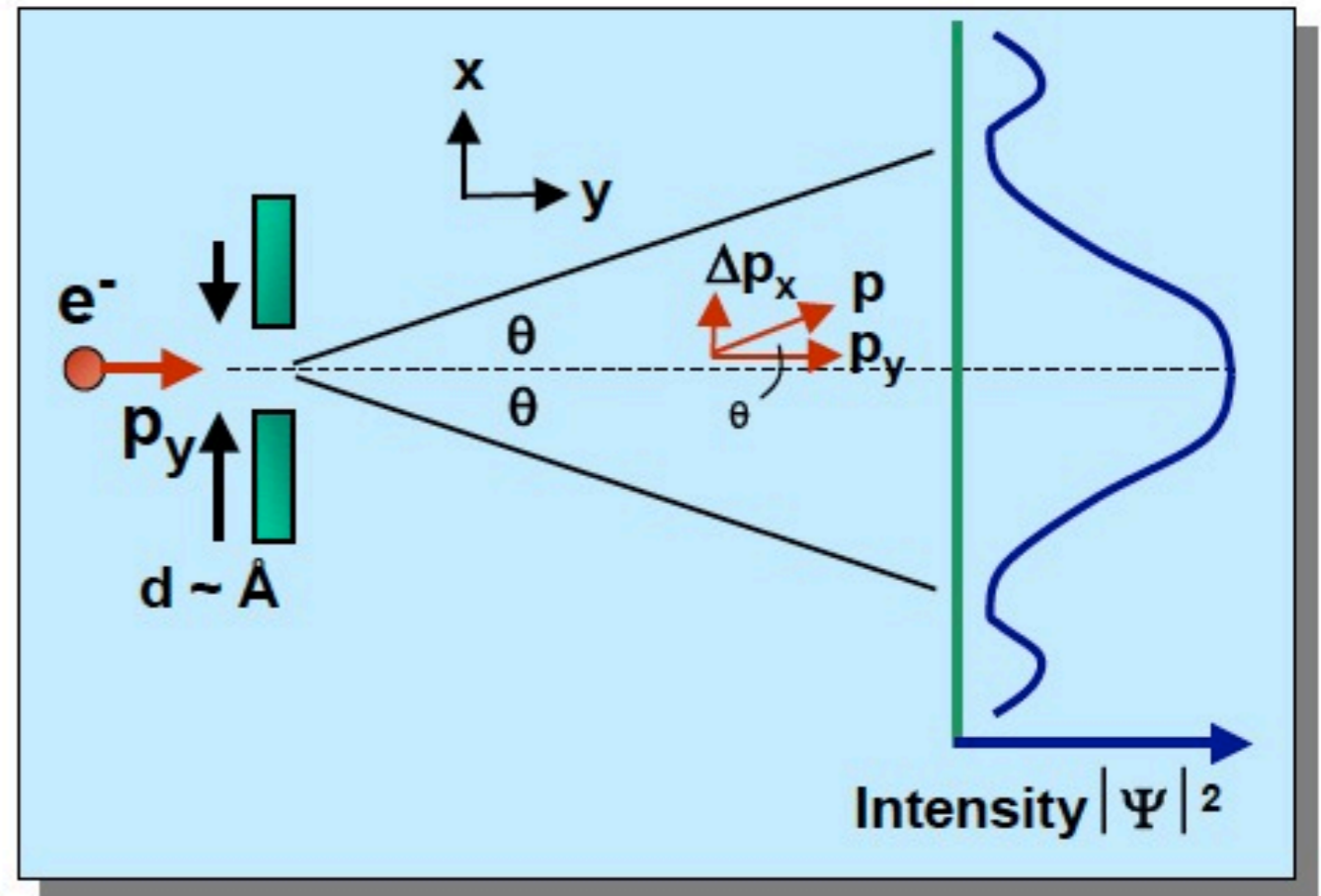
$$E = 2.05 \times 10^6 \text{ eV} = 2.05 \text{ MeV}$$

測不準原理 (Heisenberg Uncertainty Principle)

- electron single-slit diffraction

as e^- wave goes through slit

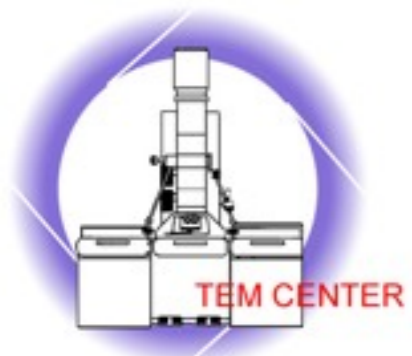
→ { uncertainty in lateral position = $d = \Delta x$
uncertainty in momentum in x -direction = Δp_x



$$\Delta p_x > p \sin \theta \quad , \quad \sin \theta = \lambda / d = \lambda / \Delta x$$

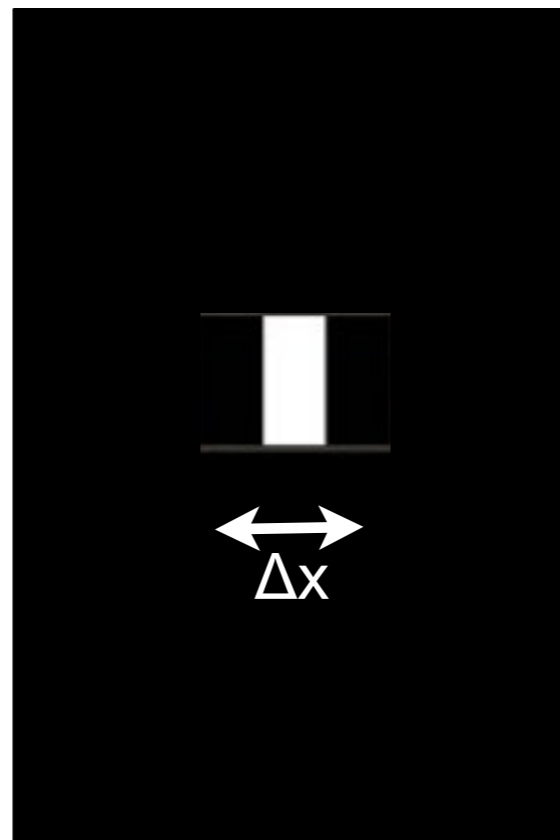
$$p = h / \lambda \quad \rightarrow \quad \Delta p_x > (h / \lambda) \sin \theta = (h / \lambda) (\lambda / \Delta x) \Rightarrow \Delta p_x \cdot \Delta x > h$$

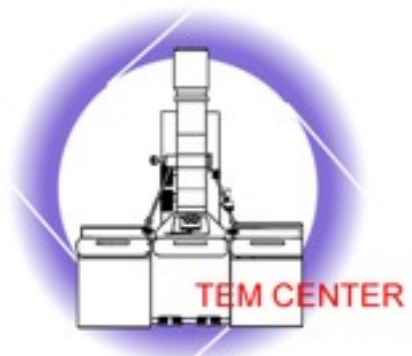
$d \downarrow \Rightarrow$ { locate the particle more precisely
greater uncertainty in momentum



Uncertainty Principle in Diffraction

NTHU





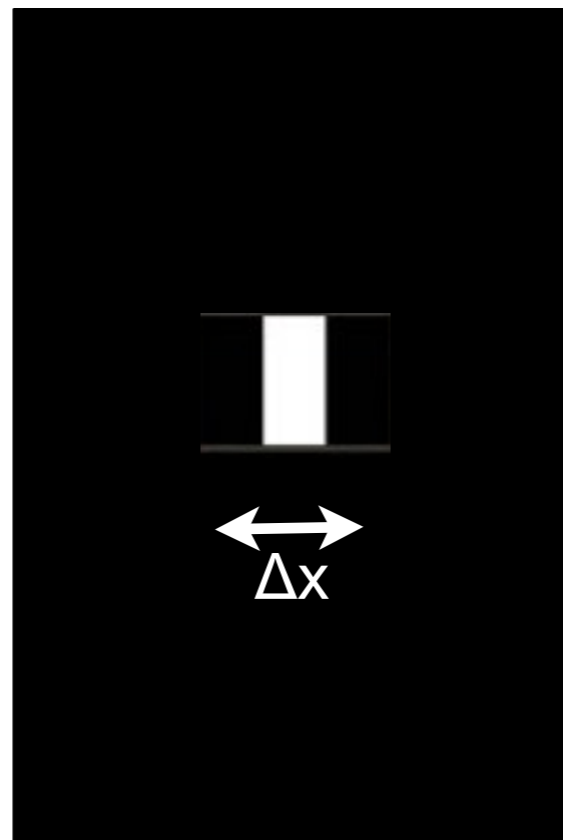
Uncertainty Principle in Diffraction

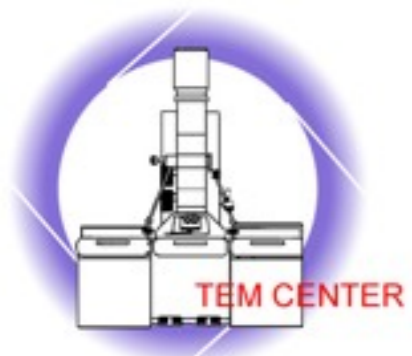
NTHU

Diffraction plane



Δp





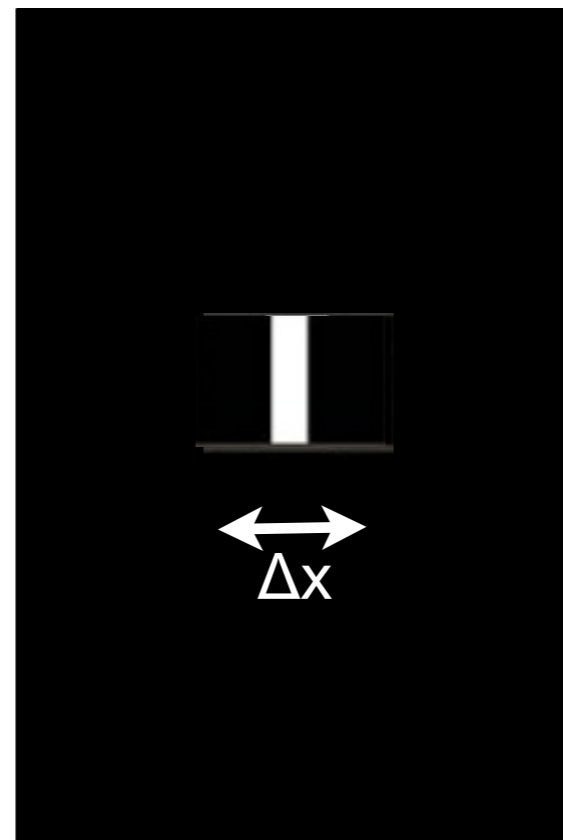
Uncertainty Principle in Diffraction

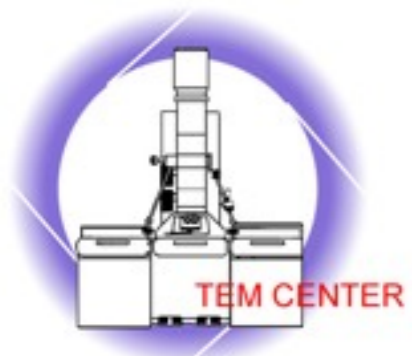
NTHU

Diffraction plane



Δp





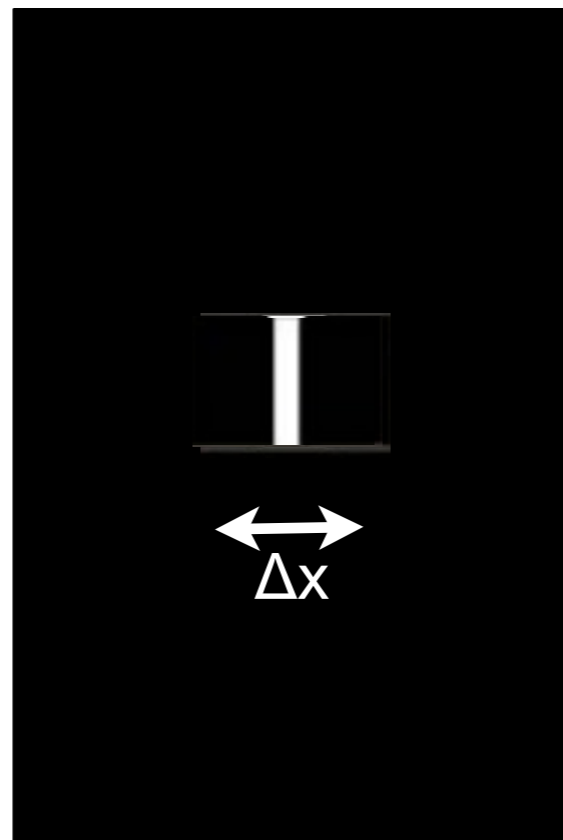
Uncertainty Principle in Diffraction

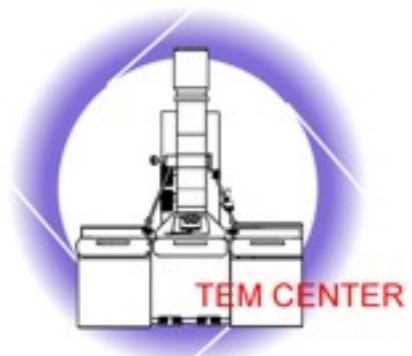
NTHU

Diffraction plane



Δp

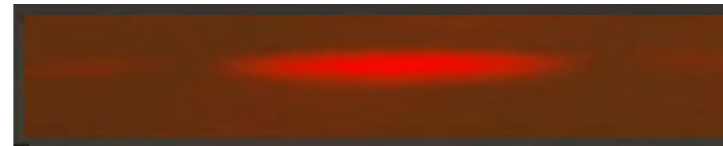




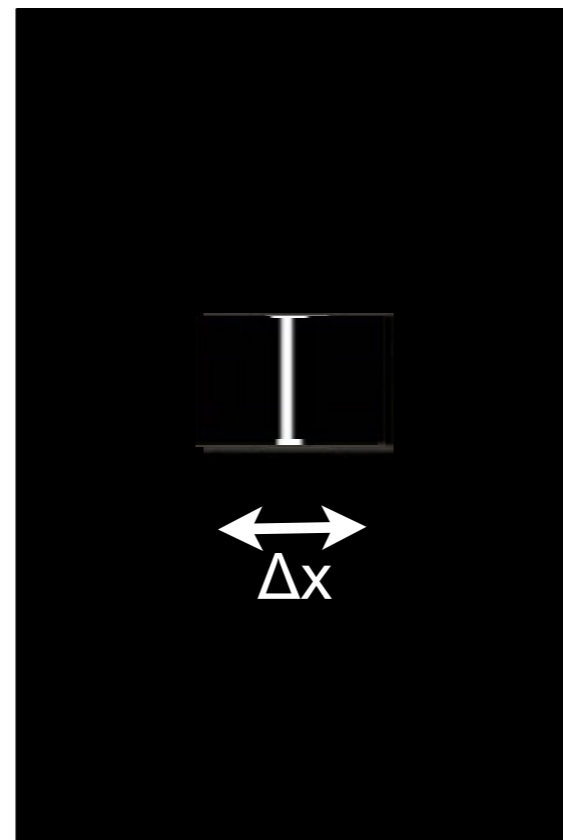
Uncertainty Principle in Diffraction

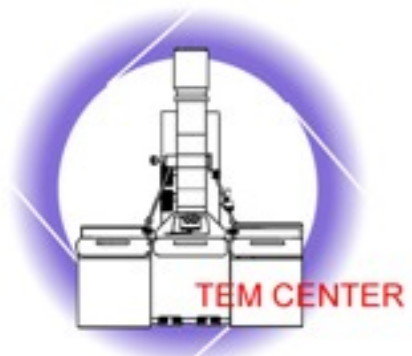
NTHU

Diffraction plane



Δp





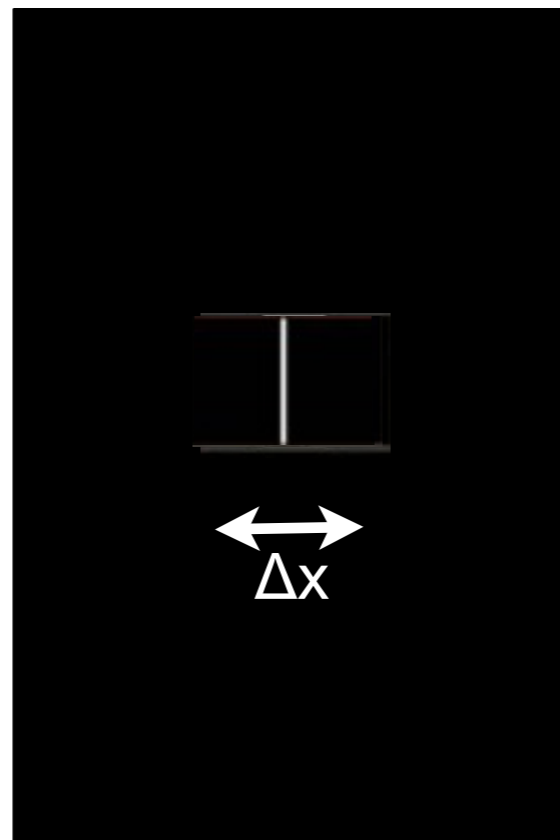
Uncertainty Principle in Diffraction

NTHU

Diffraction plane



Δp





Probability in Quantum Mechanics

NTHU

The wavefunction represents the probability amplitude for finding a particle at a given point in space at a given time. The actual probability of finding the particle is given by the product of the wavefunction with its complex conjugate (like the square of the amplitude for a complex function).

$$\Psi(x, y, z, t) = \text{probability amplitude} \quad \Psi^* \Psi = \text{probability}$$

Since the probability must be = 1 for finding the particle somewhere, the wavefunction must be normalized. That is, the sum of the probabilities for all of space must be equal to one. This is expressed by the integral

$$\int \Psi^* \Psi d\mathbf{r} = 1$$

Part of a working solution to the Schrodinger equation is the normalization of the solution to obtain the physically applicable probability amplitudes.