PHYS-3301

Lecture 5

Sep. 5, 2024

Chapter. 4
Wave & Particles II

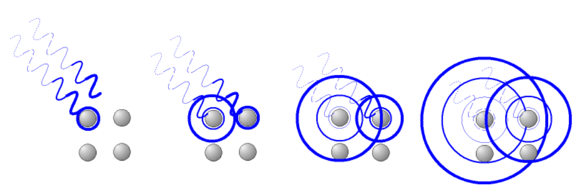
"Matter" behaving as "Waves"

Outline:

- A Double-Slit Experiment (watch "video")
- Properties of Matter Waves
- The Free-Particle Schrödinger Equation
- **Uncertainty Principle**
- **The Bohr Model of the Atom**
- **Mathematical Basis of the Uncertainty Principle – The Fourier Transform**

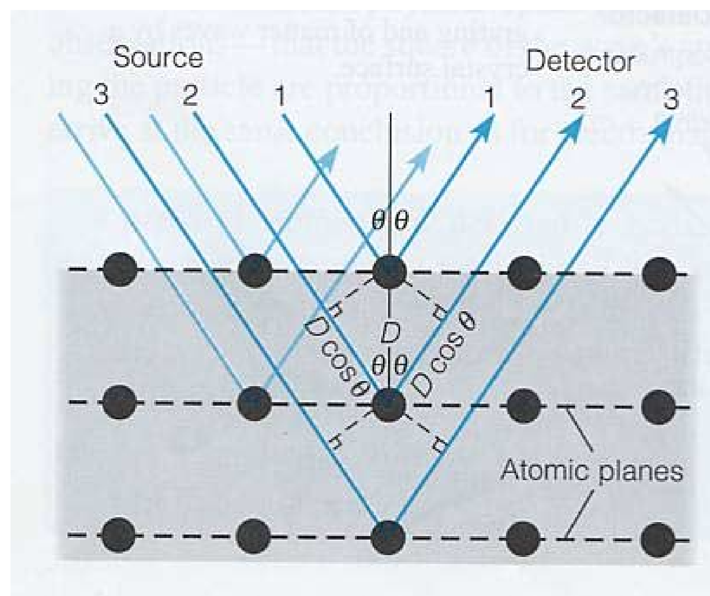
Bragg's Law

- **Bragg's law** states that when X-rays hit an atom (in a x-tal), they make the electronic cloud move as does any EM-wave. The movement of these charges re-radiates waves with the same frequency; this phenomenon is known as the Rayleigh scattering.



- These re-emitted wave fields interfere with each other either constructively or destructively, producing a diffraction pattern on a detector or film. The resulting wave interference pattern is the basis of diffraction analysis. [..excellent probe for small length scale]

Diffraction of a beam from multiple atomic planes



Bragg's Law

Derivation of Bragg's Law

Constructive interference occurs only when

$n\lambda = AB + BC$

$AB = BC$

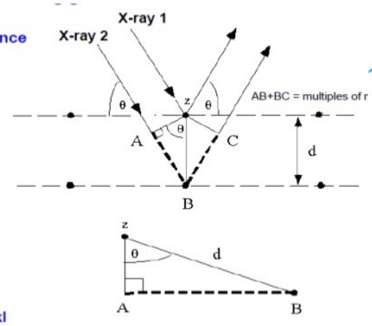
$n\lambda = 2AB$

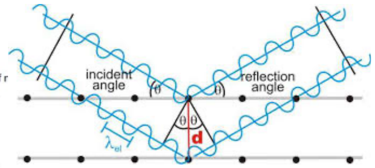
$\sin\theta = AB/d$

$AB = d\sin\theta$

$n\lambda = 2d\sin\theta$

$\lambda = 2d_{hkl}\sin\theta_{hkl}$





$$n\lambda = 2d\sin\theta,$$

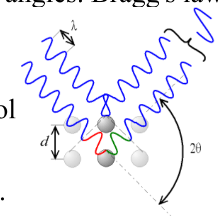
Bragg's Law

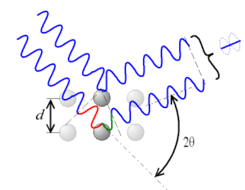
- The interference is constructive when the phase shift is a multiple of 2π; this condition can be expressed by Bragg's law,

$$n\lambda = 2d\sin\theta,$$

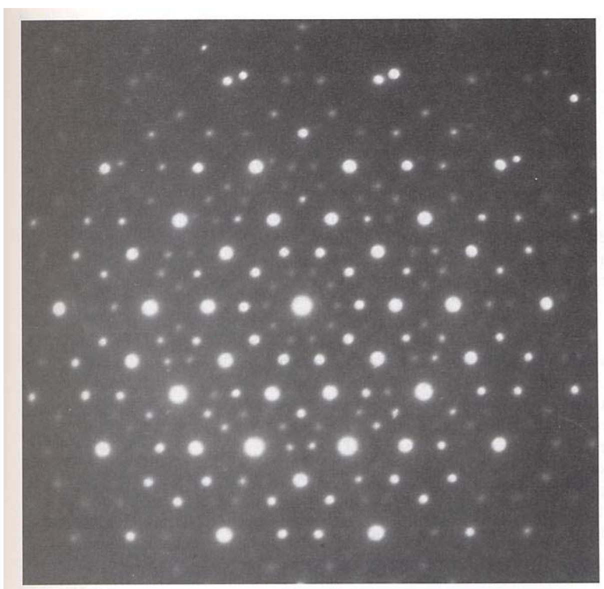
- **n** is an integer determined by the order given, **λ** is the wavelength of the X-rays, **d** is the spacing between the planes in the atomic lattice, and **θ** is the angle between the incident ray and the scattering planes.

- Bragg's Law is the result of experiments into the diffraction of X-rays off crystal surfaces at certain angles. Bragg's law confirmed the existence of real particles at the atomic scale, as well as providing a powerful new tool for studying crystals in the form of X-ray diffraction.





Electron wave diffracted by AlMn quasicrystal



De Broglie Hypothesis

The E&M waves can be described using the language of ***quantum*** particles (photons). **Q:: Can particles behave as waves?**

De Broglie (1923) suggested that a plane mono-energetic wave is associated with a freely moving particle:

$$\Psi(x) = \Psi_0 e^{i(\omega t - kx)}$$

This is a solution of the wave equation in 1-dimension:

$$\frac{\partial^2\psi}{\partial t^2} = v^2\frac{\partial^2\psi}{\partial x^2}$$

This wave travels with the ***phase*** velocity

$$v = \frac{\omega}{k}$$

We'll apply the same logic which helped us to establish the relationship between ***p*** and λ for photons:

for photon, E = pc and E = hf
hf = pc => h = pc/f = pλ so, λ = h/p

De Broglie wavelength

p - the object's m/m

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

- depends on the ***momentum*** rather then ***energy*** (e.g., for an object at rest, λ = **infinity**)

Compare with Compton wavelength of the particle

$$\lambda_C = \frac{h}{mc}$$

4.2 Properties of Matter Waves

- What properties characterize a wave?
- λ, f, v, also A that varies with position/time (i.e. (x,t))
- Wave function: we use different symbol for wave function of different kinds of wave

(1) For transverse wave on string; y(x,t)
-- string's transverse "displacement"
(2) For E&M plane wave; E(x,t) &B(x,t)
-- describe how the oscillating E- & B-field vary with (x,t)
(3) For matter wave;
$\psi(x,t)$ = probability amplitude
$|\psi(x,t)|^2$ ➔ tell us probability of finding the particle
(see next slide for some details)

Properties of Matter Waves

Amplitude = function of (x,t)

$\Psi(x,t)$

Probability Amplitude

Amplitude = function of (x,t)

$\Psi(x,t)$

***Probability* Amplitude**

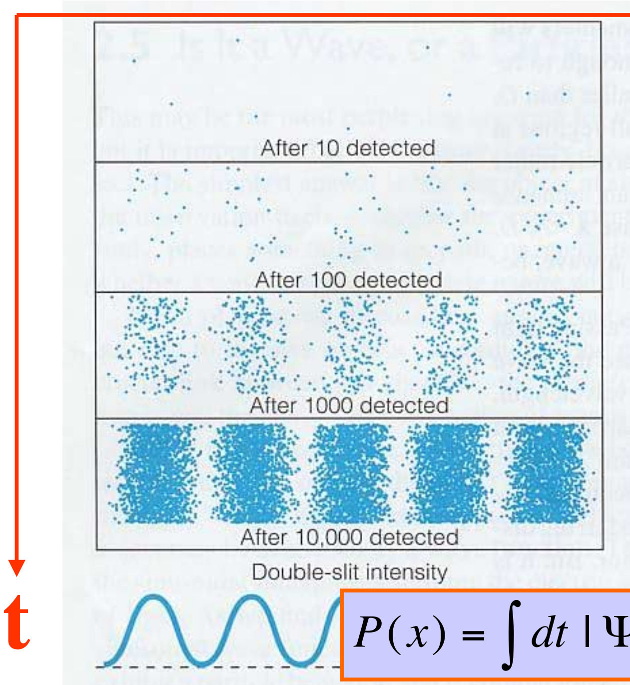
The *probability density* to find a particle at coordinate x, at time t

$|\Psi(x,t)|^2$

The *probability* to find a particle in an interval Δx, Δt

$$P = \iint dxdt\ |\Psi(x,t)|^2$$

Integrate over Δx, Δt



$$P(x) = \int dt\, |\Psi(x,t)|^2$$

4.2 Properties of Matter Waves

- **Wave length**
  - **De Broglie's hypothesis:** $\boxed{\lambda = \frac{2\pi}{k} = \frac{h}{p}}$ $\Longleftrightarrow$ $\lambda_C = \frac{h}{mc}$
  - **λ = Wavelength of matter wave**
  - **Experimentally confirmed; e.g. x-tal diffraction**
  - **de Broglie got Nobel prize in 1929**

- **Frequency (of matter waves)**
  - $f = E/h$
  - **now, it's open more convenient to express λ = *h/p* and f = *E/h* in terms of the following quantities;**
    $k = 2\pi/\lambda$ (wave number), $w = 2\pi/T$ (angular frequency)
  - **Another convenient definition: $\hbar = h/2\pi = 1.055 \times 10^{-34}$ Js**
  - **express the fundamental wave-particle relationship as**

$$\boxed{\vec{p} = \hbar\vec{k}} \qquad \boxed{E = \hbar\omega}$$

Properties of Matter Waves

De Broglie (1929)

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

Frequency $\boxed{f = \frac{E}{h}}$

Properties of Matter Waves

Speed $\boxed{v = f\lambda}$

It does give the wave speed
v = (E/h)(h/p) = E/p
c.f. for photon, E = pc

BUT
***v* is NOT the velocity of the massive particle, it's the velocity of the Matter wave**

Electromagnetic waves (light) → Particles (photons)

?

Waves ← Massive Particles

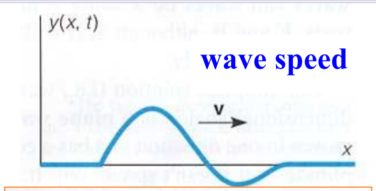
How does the Probability Wave Move?

Equation of Motion for ψ ?

The Free-Particle Schrodinger Wave Equation

[Q] How do we determine the $\psi(x,t)$ of a matter wave?

Waves on a string



$$v^2 \frac{\partial^2 y(x,\ t)}{\partial x^2} = \frac{\partial^2 y(x,\ t)}{\partial t^2}$$

Waves on a string

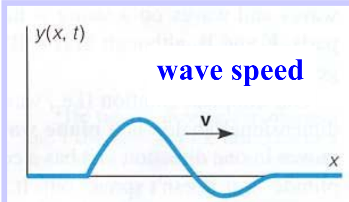


Figure 3.9 A wave disturbance on a string.

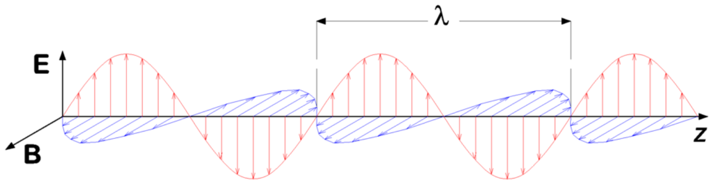
$$v^2 \frac{\partial^2 y(x,\ t)}{\partial x^2} = \frac{\partial^2 y(x,\ t)}{\partial t^2}$$

Solution = function

"Plane Wave"

$$y(x,\ t) = A \sin(kx - \omega t) \quad \text{where} \quad \frac{\omega}{k} = v$$

E&M Wave

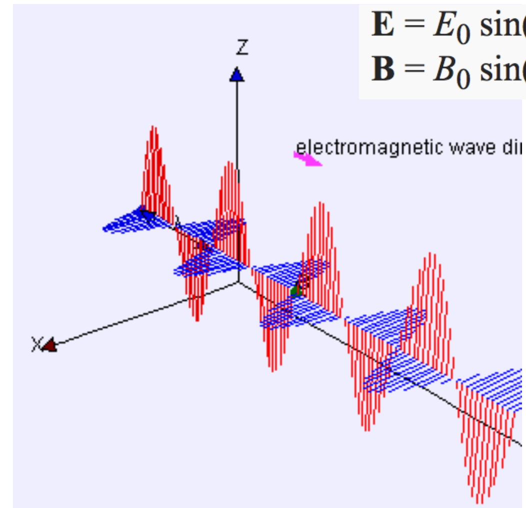


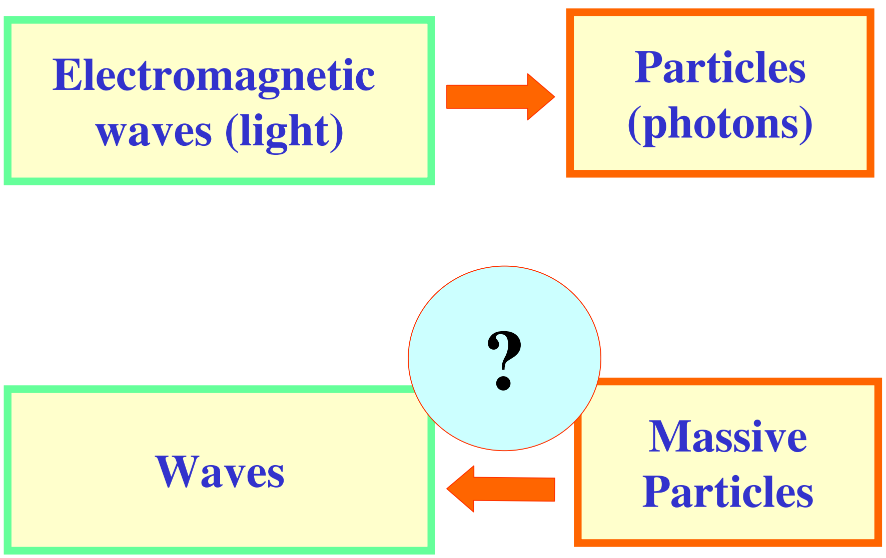
$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} - \nabla^2 \mathbf{E} = 0$$
$$\frac{1}{c^2}\frac{\partial^2 \mathbf{B}}{\partial t^2} - \nabla^2 \mathbf{B} = 0$$

$$\mathbf{E} = E_0 \sin(-\omega t + \mathbf{k}\cdot\mathbf{r})$$
$$\mathbf{B} = B_0 \sin(-\omega t + \mathbf{k}\cdot\mathbf{r})$$

E&M Wave

$$\mathbf{E} = E_0 \sin(-\omega t + \mathbf{k}\cdot\mathbf{r})$$
$$\mathbf{B} = B_0 \sin(-\omega t + \mathbf{k}\cdot\mathbf{r})$$





4.3 The Free-Particle Schrodinger Eq.

[Q] How do we determine the ψ(x,t) of a matter wave?

[A] Matter Waves

-- wave eq. obeyed by matter waves ➔ Schrödinger eq.

-- for free particle, in the absence of external forces,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial \Psi(x,t)}{\partial t} \qquad v^2\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{\partial^2 y(x,t)}{\partial t^2}$$

[Q] Schrodinger eq. is "complex". Matter wave is not "real"?

[A] Reason for "i" :: NOT matter waves are "unreal"

BUT they can't be represented by a single real function !!

real now!!

e.g. like E&M waves, 2 parts (E & B) and a complex function, carrying twice the info. of a real one.

===> In E&M, we could treat E & B as a single complex unit by including "i" w/o making either field "unreal" ===> Combined WF, G = E + iCB

(Wave Function)^2 = Probability Density

The Free-Particle Schrodinger Wave Equation

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

$\psi(x,t)$ **Probability Wave Function**

$\psi^*(x,t)\psi(x,t) = |\psi(x,t)|^2$ **Probability Density**

$\psi(x,t)$ **a <u>complex</u> function**