Matter waves

We mentioned de Broglie's hypothesis last time
(1923)

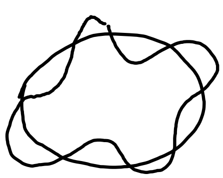
particles also exhibit wave properties

$$\begin{cases} f = \dfrac{E}{h} \\ \lambda = \dfrac{h}{p} \end{cases}$$

(as we saw light waves exhibit particle-like properties $E = hf$ & $p = \frac{h}{\lambda}$)

This was used to explain the Bohr quantization condition

angular momentum $L = \frac{nh}{2\pi} = n\hbar \quad (\hbar \equiv \frac{h}{2\pi}) \quad n = 1, 2, 3 \ldots$



$$2\pi r = n\lambda \Rightarrow \lambda = \frac{2\pi r}{n}$$

$$L = rp = r \cdot \frac{h}{\lambda} = r \cdot \frac{h}{\frac{2\pi r}{n}} = n\frac{h}{2\pi}$$

which was used by Niels Bohr to derive energy levels for hydrogen atoms.

We will come back to Chapter 5 after we study quantum mechanics for 1d, 2d & 3d.

At that time even de Broglie did not know what is the nature of "the wave", it was referred to as the "matter waves".

But why wasn't such a wave observed before?

Ans. wavelength too small.

Example 6.1 e^- with kinetic energy $K = 10, 100, 10^3, 10^4 eV \Rightarrow \lambda = ?$

Use non-relativity as $K \ll MeV$. $K = \frac{p^2}{2m}$. $p = \sqrt{2mK}$.

$$\lambda = \frac{h}{\sqrt{2mK}} = \frac{hc}{\sqrt{2mc^2K}} = \frac{1240\ eV \cdot nm}{\sqrt{2 \times 0.511 \times 10^6\ eV \cdot 100\ eV}} = \frac{1240\ nm}{\sqrt{1.022} \times 10^4} \cong 0.12\ nm$$

e.g. $K = 100\ eV$

K (eV)	10	100	1000	10^4
λ (nm)	0.39	0.12	0.039	0.012

$\lambda \propto \frac{1}{\sqrt{m}}$

↳ so neutron has even smaller wavelength

cf. X-rays

↳ comparable to wavelength of X-rays. ⟹ would be used for crystals too.

* But requires very good vacuum to avoid scattering by gas ($K \sim 100$ eV)

I.

1927 Clinton Davisson & Lester Germer : diffraction of electron waves

e.g. $K = 54$ eV at nickel crystal. ⟹ agrees

1927 G. P. Thomson : diffraction of e^- transmitted thru thin metal foils

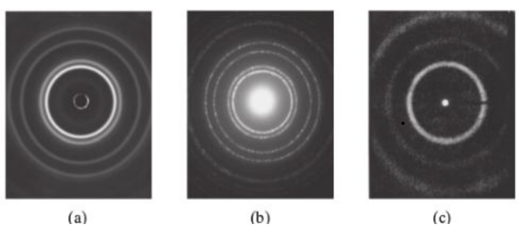
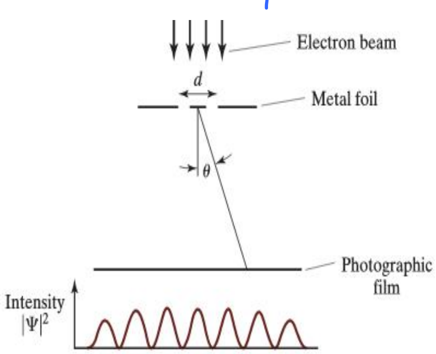


FIGURE 6.3
Diffraction rings produced by diffraction of waves in polycrystalline metal samples with **(a)** X-rays, **(b)** electrons, **(c)** neutrons.

II. double-slit experiment for e^-



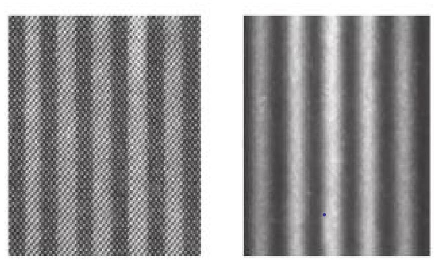


FIGURE 6.4
Two-slit interference patterns produced by light and electrons.

Q: which way did the e^-'s go thru?

Ans: if you try to use light to see which slit e's go thru, interference pattern disappears!

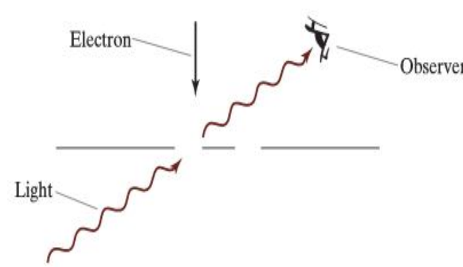


FIGURE 6.7
To find out which slit the electron passes through, we shine a narrow beam of light through one of the slits.

Using e^- for interference, $\lambda_{el} \simeq d$. $P_{el} = \frac{h}{\lambda_{el}} \approx \frac{h}{d}$

As you need to use light w. wave length $\lambda_r \leq d$

$\Rightarrow P_r = \frac{h}{\lambda_r} \gtrsim \frac{h}{d}$ $\Rightarrow$ detection of e^- will change e^-'s momentum, smearing interference pattern.

$\Rightarrow$ It is not possible to measure position x and momentum p precisely w/o change one or the other. Heisenberg's uncertainty principle

$\Delta x \, \Delta p \geq \frac{\hbar}{2}$. [later]

$\Longrightarrow$ what was detected is the intensity (of photons or e^-'s)

Q1: what is the nature of the matter wave? Probability amplitude

Q2: what is the equation that governs the wave? Schrödinger's wave equation

Quantum wave function

Consider $\mathcal{E}$ electric field $\mathcal{E}(r,t)$

$\Rightarrow$ energy in volume dV at $\vec{r}$: E (in dV at r) $= \varepsilon_0 |\mathcal{E}(r,t)|^2 dV$

(# of photons in dV at r) $\sim \frac{E}{hf} \propto |\mathcal{E}(r,t)|^2 dV$

$P(r)$

$\hookrightarrow$ probable # of photons

Max Born: matter wave $\Psi(\vec{r},t)$

$$|\Psi(\vec{r},t)|^2 \, dV = (\text{probable \# of } e^- \text{ in } dV \text{ at } \vec{r}) \quad P$$

this quantum wave fcn $\Psi(\vec{r},t)$ is in general complex: $\Psi = \Psi_{real} + i\,\Psi_{imag}$

$i = \sqrt{-1}$, $|\Psi|^2 = \Psi_{real}^2 + \Psi_{imag}^2$

$\longrightarrow$ answers Q1.

Ans to Q2: Schrödinger's equation e.g. $i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r},t) + V(\vec{r})\,\Psi(\vec{r},t)$

Sinusoidal Waves

$$y(x,t) = A \sin 2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right) \qquad \Rightarrow \quad f = \frac{1}{T}$$

$$= A \sin(kx - \omega t) \qquad \omega = 2\pi f \text{ angular freq}$$

(phase) velocity $v = \dfrac{\lambda}{T} = \lambda f = \dfrac{\omega}{k}$

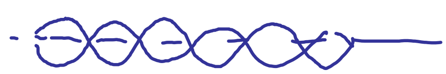
$\Downarrow$

de Broglie relation:
$$\begin{cases} E = hf \\ p = \dfrac{h}{\lambda} \end{cases}$$

Recall superposition principle: e.g. create a standing wave out of two counter-propagating traveling waves.

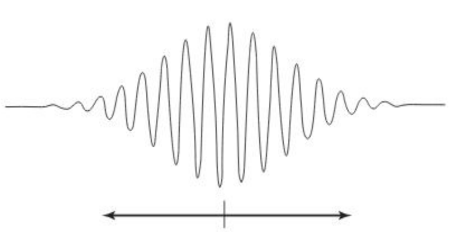
$y_R(x,t) = A \sin(kx - \omega t)$ $\rightarrow$ $+$ $\leftarrow$ $y_L(x,t) = A \sin(kx + \omega t)$

$y(x,t) = y_R(x,t) + y_L(x,t) = 2A \sin kx \cos \omega t$



Wave packets & Fourier analysis

In the above examples, the waves are infinite in extent. Typical waves e.g. sound wave, seismic waves, ... are finite in extent. These come in the form of a wave packet.



Consider such a wave packet on the left. In order to make the wave confine mostly in a region $[-\Delta x, \Delta x]$. we shall see that the spread in k i.e. Δk satisfy

$$\Delta k \approx \frac{1}{\Delta x}$$ [so if $\Delta k = 0 \Rightarrow \Delta x = \infty$, or $\Delta x = 0 \Rightarrow \Delta k = \infty$]

Using momentum spread $\Delta p = \hbar \Delta k$, we have

$\Delta p \approx \dfrac{\hbar}{\Delta x}$, which is the uncertainty principle $\boxed{\Delta x \, \Delta p \geq \frac{\hbar}{2}}$

The mathematics that we need is the Fourier analysis.

Fourier series

Consider only even function for simplicity $f(x) = f(-x)$

For a even periodic function $f(x)$ it can be expressed as a sum of a series

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{2\pi n}{\lambda} x\right) = \sum_{n=0}^{\infty} A_n \cos k_n x. \qquad k_n = \frac{2\pi}{\lambda} n = \frac{1}{\lambda_n} \qquad \left(f(x) = f(x+\lambda) \right)$$

Fourier sum/series   Fourier coeff.

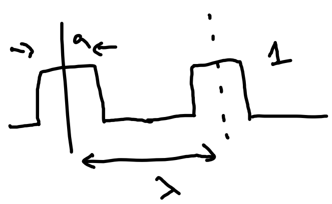
$$\lambda_n = \frac{\lambda}{n} \quad (n \neq 0)$$

$n=1$: $\lambda_n = \lambda$ fundamental

$n>1$: λ_n higher harmonics

$$A_n = \frac{2}{\lambda}\int_0^{\lambda} dx \cos\frac{2\pi n}{\lambda}x \, f(x) \qquad A_0 = \frac{1}{\lambda}\int_0^{\lambda} dx \, f(x)$$

e.g.



$$A_n = \frac{2}{\lambda}\left(\int_0^{\frac{a}{2}} + \int_{\lambda-\frac{a}{2}}^{\lambda}\right) \cos\frac{2\pi n}{\lambda} x$$

$$= \frac{2}{\lambda}\left(\frac{\lambda}{2\pi n} \sin\frac{2\pi n}{\lambda} x \Big|_0^{\frac{a}{2}} + \Big|_{\lambda-\frac{a}{2}}^{\lambda} \right)$$

$$= \frac{2}{\lambda}\frac{\lambda}{2\pi n}\left(\sin\frac{\pi n a}{\lambda} - \sin\frac{2\pi n}{\lambda}\left(\lambda - \frac{a}{2}\right)\right)$$

$$= \frac{2}{\pi n}\sin\frac{\pi n a}{\lambda} \qquad n = 1, 2, \ldots$$

$$\left(\text{for } n=0 \quad A_0 = \frac{a}{\lambda}\right)$$

In general if we do not restrict to even functions, then we have

in general
$$f(x) = \sum_n \left(A_n \cos\frac{n\pi x}{\lambda} + B_n \sin\frac{n\pi x}{\lambda} \right)$$

Fourier integrals

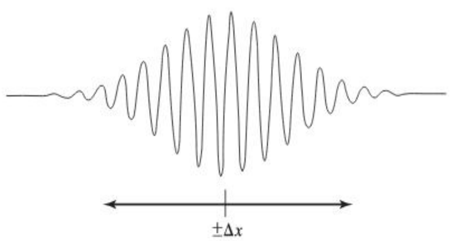
For functions that are not periodic, we can think of their period (in space) $\lambda \to \infty$

Then for even function

$$f(x) = \int_0^{\infty} A(k) \cos kx \, dk \qquad A(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} f(x) \cos kx \, dx$$

Fourier transform

↳ Look at a wave packet centered on the origin : $\lambda \pm \Delta\lambda$



Focus on two extremes $\lambda - \Delta\lambda$ & $\lambda + \Delta\lambda$.

Spread of k = ? $k = \frac{2\pi}{\lambda}$, $\Delta k = \left|\frac{dk}{d\lambda}\right| \Delta\lambda$

$$\boxed{\Delta k = \frac{2\pi}{\lambda^2}\Delta\lambda}$$

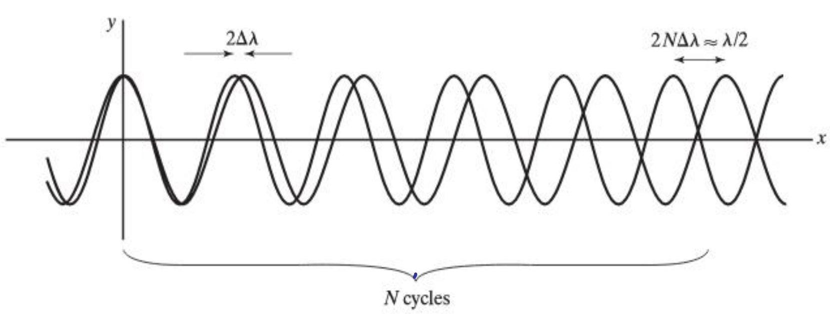
At about $N\lambda$ from origin, i.e. $x = N\lambda$

the two waves differ in positions of peaks $2N\Delta\lambda$ and destructively interfere

if $2N\Delta\lambda \approx \lambda/2$ (out of phase) $\left[N \approx \frac{\lambda}{4\Delta\lambda}\right]$

$\Rightarrow$ Half-width of packet $\Delta x \approx N\lambda = \frac{\lambda^2}{4\Delta\lambda} = \frac{1}{4}\frac{2\pi}{\Delta k}$

$\Rightarrow$ $\Delta x \Delta k \approx \pi/2$ of order 1.



Δx is usually defined as

$$\Delta x = \sqrt{\langle (x - x_0)^2 \rangle}$$

$$x_0 = \langle x \rangle.$$

$\langle \dots \rangle \Rightarrow$ average

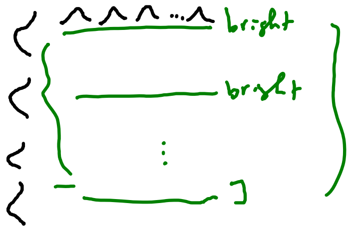
$$\Rightarrow \Delta x \Delta k \geq \frac{1}{2}$$

Similar analysis leads to $\Delta\omega\,\Delta t \geq \frac{1}{2}$

Example 6.2

A TV picture, composed of 525 horizontal lines, refreshes 30 times a second. Hence, each line is drawn across the screen in $1/(30 \times 525)$ s $= 6.3 \times 10^{-5}$ s. What is the approximate range of frequencies Δf at which a TV transmitter must be able to broadcast, if the horizontal and vertical resolutions in the TV picture are to be about the same?

vertical resolution



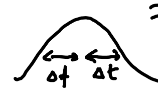
30 times a second

$\Rightarrow$ each line drawn 6.3×10^{-5} sec

Want horizontal resolution = vertical

$$\Rightarrow \quad 2\Delta t \approx \frac{6.3 \times 10^{-5}\ \text{sec}}{525} = 1.2 \times 10^{-7}\ \text{s}$$

$2\Delta t$



$$\Delta\omega \geq \frac{1}{2\Delta t} \approx 8.3 \times 10^{6}\ \text{s}^{-1}, \quad \Delta f = \frac{\Delta\omega}{2\pi} \gtrsim 1.3 \times 10^{6}\ \text{H}$$

$$\Rightarrow \text{band width } 2\Delta f = 2.6 \times 10^{6}\ \text{Hz}$$

Uncertainty principles / relations

$\Delta x\,\Delta p \geq \frac{\hbar}{2}$ $\rightarrow$ If a particle's position is uncertain to within $\pm\Delta x$ and its momentum is $\pm\Delta p$

Then uncertainty principle says $\Delta x\,\Delta p \geq \frac{\hbar}{2}$

Since $p = \frac{h}{\lambda} = \hbar k$, $\Delta p = \hbar\Delta k$

From Fourier analysis we have $\Delta x\,\Delta k \geq \frac{1}{2}$

Thus $\Delta x\,\Delta p = \Delta x\,\hbar\Delta k \geq \frac{\hbar}{2}$.

[classical mechanics assume that x & p can be measured ~~as~~ to any accuracy]

$\Delta E\,\Delta t \geq \frac{\hbar}{2}$ From $\Delta t\,\Delta\omega \geq \frac{1}{2}$ and $E = hf = \hbar\omega$

$\Delta t\,\Delta E \geq \frac{\hbar}{2}$ [time-energy uncertainty relation]

ΔE is uncertainty in a particle's energy and Δt is the time spent by a wave packet at some position.

Δt can also be thought of as time it takes for the system to change substantially its energy ΔE.

Example 6.3

The position x of a 0.01-g pellet has been carefully measured and is known within $\pm 0.5\,\mu$m. According to the uncertainty principle, what are the minimum uncertainties in its momentum and velocity, consistent with our knowledge of x?

$\Delta x\, \Delta p \geq \frac{\hbar}{2}$
$m \Delta v$

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{1.05\times 10^{-34}\ J\cdot s}{2\cdot 0.5\times 10^{-6}\ m} \sim 10^{-28}\ kg\cdot\frac{m}{s}$$

$$\Delta v = \frac{\Delta p}{m} \gtrsim \frac{10^{-28}\ kg\,\frac{m}{s}}{0.01\times 10^{-3}\ kg} \sim 10^{-25}\ \frac{m}{s}$$

Example 6.4

An electron is known to be somewhere in an interval of total width $a \approx 0.1$ nm (the size of a small atom). What is the minimum uncertainty in its velocity, consistent with this knowledge?

useful numbers

$$\boxed{\begin{array}{l}\hbar c \approx 200\ eV\cdot nm \\ hc \cong 1240\ eV\cdot nm\end{array}}$$

$\Delta x \leq \frac{a}{2} \sim 0.05\,nm$ $\qquad \Delta p \gtrsim \frac{\hbar}{a}$

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{2m\Delta x} \approx \frac{\hbar}{ma} \sim \frac{1.05\times 10^{-34}\ J\cdot s}{9.11\times 10^{-31}\ kg\cdot 10^{-10}\ m} \sim 1.15\times 10^{6}\ \frac{m}{s}$$

↳ This example shows that a particle confined in a small region cannot be exact at rest!

On average kinetic energy $\langle K\rangle = \langle \frac{p^2}{2m}\rangle \gtrsim \frac{(\Delta p)^2}{2m} \sim \frac{\hbar^2}{2ma^2}$

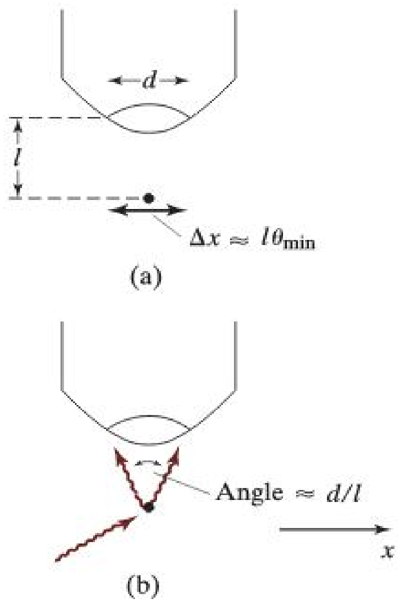
$\Rightarrow$ zero point energy

Example 6.5

What is the minimum kinetic energy of an electron confined in a region of width $a \approx 0.1$ nm, the size of a small atom?

$$\langle K \rangle \sim \frac{\hbar^2}{2ma^2} \sim \frac{(1.05\times10^{-34}\,\mathrm{J\cdot s})^2}{2\cdot 9.11\times10^{-31}\,\mathrm{kg}\cdot(10^{-10}\,\mathrm{m})^2} \sim 6.05\times10^{-19}\,\mathrm{J} \sim 3.78\,\mathrm{eV}$$

Heisenberg's microscope — an thought. experiment



classical physicist tries to disprove uncertainty relation

① Find position x of particle → use microscope whose resolution is limited by diffraction of light

$\theta_{\min} \approx \frac{\lambda}{d}$ λ : wavelength of light

d : diameter of lens

Δx : uncertainty in position

$\Delta x \approx l\,\theta_{\min} \sim \frac{l\lambda}{d}$

→ make Δx as small by using as small λ !

② momentum?

to measure speed : need to have light collide with particle

⇒ light scattered and direction is uncertain by an angle $\sim \frac{d}{l}$ ⇒ x component of photon uncertain $\left(\frac{h}{\lambda}\right)\frac{d}{l} \lesssim \Delta p_x$

· want to make Δp_x small ⇒ large λ !

So $\Delta p_x \Delta x \gtrsim h$ cannot beat uncertainty principle.

uncertainty principle also applies to other direction

$\Delta y\,\Delta p_y \gtrsim \hbar/2$, $\Delta z\,\Delta p_z \gtrsim \hbar/2$

Example 6.6

Many excited states of atoms are unstable and decay by emission of a photon in a time of order $\Delta t \approx 10^{-8}$ s. What is the minimum uncertainty in the energy of such an atomic state?

$$\Delta E \geq \frac{\hbar}{2\Delta t} \sim \frac{1.05 \times 10^{-34}\ \text{J}\cdot\text{s}}{2 \cdot 10^{-8}\ \text{s}} \sim \frac{5 \times 10^{-27}\ \text{J}}{1.6 \times 10^{-19}\ \text{eV}} \sim 3 \times 10^{-8}\ \text{eV}$$