Quantum Physics 1
Class 6

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Schrödinger Wave Equation

Last time :

Heisenberg uncertainty principle :

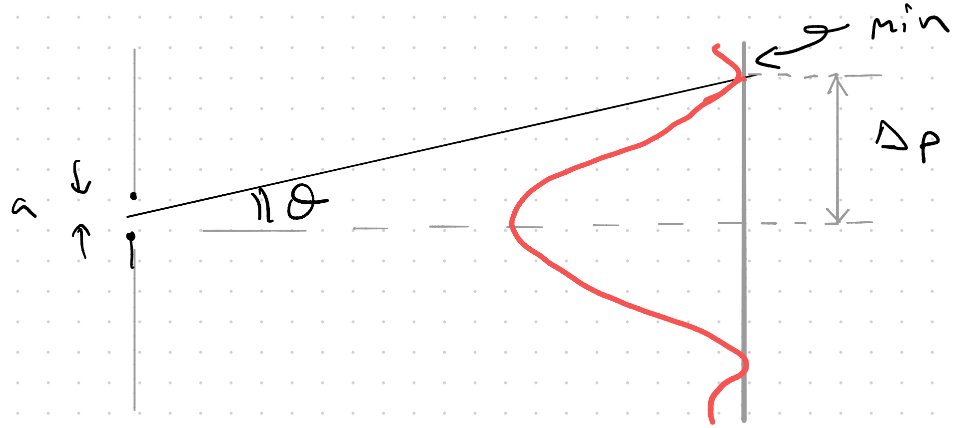
position & momentum.

$$\boxed{\Delta x \, \Delta p \geq \hbar/2}$$

$\hbar \equiv h/2\pi$

$$\boxed{\Delta x \, \Delta p \sim h}$$

("Rough" from last class)



$\Delta y = a$; $\frac{\Delta p}{p} = \sin\theta = \frac{\lambda}{a}$ $(m=1)$

$$\therefore \Delta y \, \Delta p = a \frac{p\lambda}{a} = p\lambda = \frac{h}{\lambda} \cdot \lambda = h$$

$$\boxed{\Delta y \, \Delta p \approx h}$$

Example of Uncertainty Relation : $\Delta x \Delta p \geq \frac{\hbar}{2}$

◉ Electron confined to a one-D crystal of size 10 nm.

Find : (i) Minimum uncertainty in velocity Δv ?

(ii) Minimum uncertainty in kinetic energy, ΔE

Soln: $\Delta x \Delta p = \hbar/2$

(i) $\Delta p = \frac{\hbar}{2} \cdot 10^9$

$$\Delta v = \frac{\hbar}{2} \cdot 10^9 \, \frac{1}{9.1 \times 10^{-31}} = \frac{6.62 \times 10^{-34} \cdot 10^9}{2 \times 9.10 \times 10^{-31}}$$

$$= 0.37 \times 10^6 \text{ m/s}$$

$$\Delta v = 3.7 \times 10^5 \text{ m/s}$$

Consider: $\bar{v} = 10^6$ m/s

(average velocity)

(ii) then $E = \frac{p^2}{2m}$; $\delta E = \frac{p \, \delta p}{m}$

$$\Delta E = \frac{p \Delta p}{m} = \frac{m v \Delta p}{m}$$

$$= v \Delta p$$

$$= 10^6 \left(\frac{\hbar}{2} \cdot 10^9 \right)$$

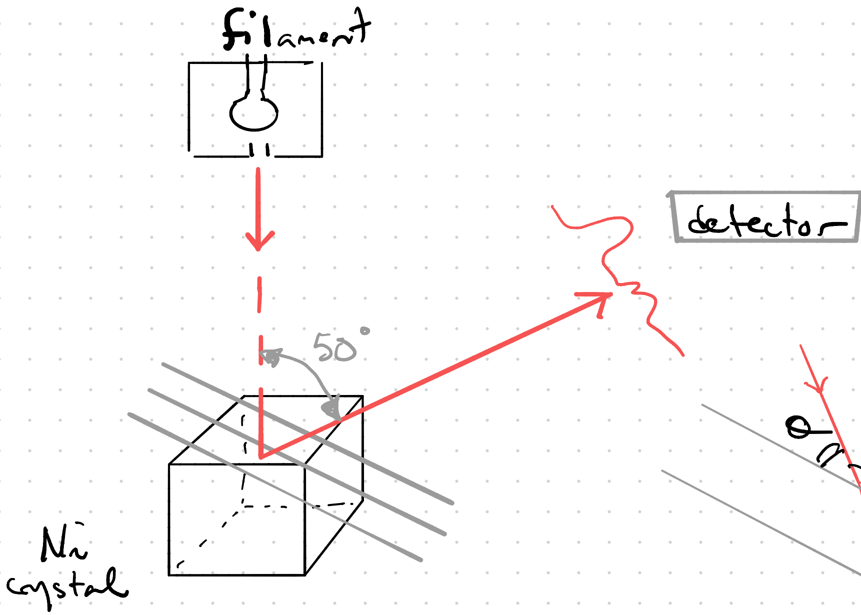
$$\Delta E = \frac{10^6 \cdot 6 \times 62 \times 10^{-34} \times 10^9}{2 \times 2\pi}$$

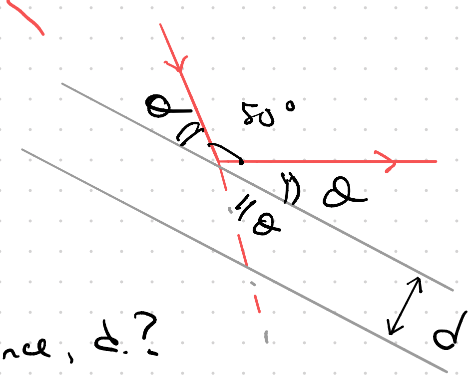
$$= 0.53 \times 10^{-19} \text{ J}$$

$$= \frac{0.53 \times 10^{-19} \text{ J}}{1.6 \times 10^{-19} \, [\text{J/eV}]}$$

$$\Delta E = 0.33 \text{ eV}$$

- If particles are waves and they can diffract, they should also interfere.
  - ~ years after de Broglie there was an accidental discovery! In the lab of Davisson and Germer (1927).
- e^- beam incident on Ni surface.





What is the inter-layer distance, d.?

** Measure peak intensity.

@ $2\theta = 180 - 50 = 130^\circ$

$\Rightarrow \theta = 65^\circ$

$$\lambda\,[\text{Å}] = \sqrt{\frac{150}{E\,[\text{eV}]}} = \sqrt{\frac{150}{54}} = 1.67\ \text{Å}$$

$$= 0.167\ \text{nm}$$

Consider: $\lambda\,[nm] = \sqrt{\dfrac{1.5}{E\,[eV]}}$

$\therefore \quad 2d\sin\theta = n\lambda \quad ; \quad n = 1$

$$\boxed{d = \frac{\lambda}{2\sin 65} = 0.92\,\text{Å}}$$

$\boxed{\text{In-class 6-1 \& 6-2}}$

from crystal

compare to photon

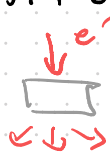
Types of e^- Scattering

i) Transmission e^- microscopy (TEM)

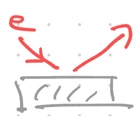
ii) Reflection high-energy electron diffraction (RHEED)

iii) Low-energy electron diffraction (LEED)

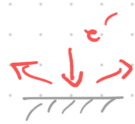
e^- Energy: (i) 100 – 300 keV



ii) 5 - 30 keV



iii) 50 - 200 eV



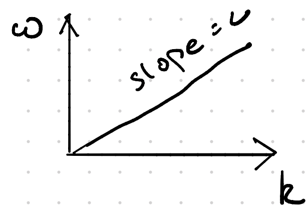
What about a mathematical description of the wave behaviour? A Wave equation?

** Recall for light:

$$\xi = A e^{i(kx - \omega t)} \quad ; \quad \text{energy} \propto |A|^2$$

$$\frac{\partial^2 \xi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \xi}{\partial t^2} \quad \text{w/t solution} \sim e^{i(kx - \omega t)}$$

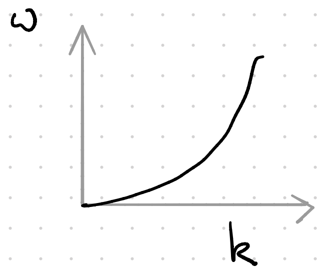
w/t $\omega = ck$



from Einstein, $E = h\nu$
$= \hbar \omega$
$\therefore E \propto k$

Now recall: $p = \frac{h}{\lambda} = \hbar k \quad ; \quad \hbar \equiv \frac{h}{2\pi}$

& $\omega = \frac{E}{\hbar} = \frac{p^2}{2m\hbar} = \frac{\hbar k^2}{2m}$



$\left\{ E = \hbar\omega = \frac{mv^2}{2} = \frac{p^2}{2m} \; ; \; p = \frac{h}{\lambda} \right\}$ aside.

consider:

$$\frac{\partial \psi^2(x,t)}{\partial x^2} = \frac{1}{v_0^2}\frac{\partial^2 \Psi(x,t)}{\partial t^2}, \quad \& \ \Psi \sim e^{i(kx-\omega t)}$$

$$\Rightarrow \quad -k^2 e^{i(kx-\omega t)} = -\frac{1}{v_0^2}\omega^2 e^{i(kx-\omega t)}$$

$$k^2 = \frac{\omega^2}{v_0^2} = \frac{\hbar^2 k^4}{4m^2 v_0^2}$$

$$\omega^2 = \frac{\hbar^2 k^4}{4m^2}$$

$$\omega = \frac{\hbar k^2}{2m}$$

recall: classically $F = m\frac{d^2 x^2}{dt^2}$; $x = x(t)$

w/ solutions: $\sin(kx-\omega t)$

$\cos(kx-\omega t)$

$\vdots$

$\& \quad E = \frac{p^2}{2m}$

In-class 6.3

Classical $\longrightarrow$ Quantum

{ Schrödinger's Guess }

$$p \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \quad ; \quad E \rightarrow i\hbar \frac{\partial}{\partial t}$$

Schrödinger Equation:

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

For particle in free space!!!

In general, we can include a potential;

classical: $\frac{p^2}{2m} + V(x) = E$

S.E.:

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

$\Psi(x,t) \equiv$ probability amplitude of finding particle at x, t

NB i) $\Psi(x,t)$ is a complex function
does not directly correspond to something we can measure.

ii) $\Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2$ Probability density

iii) $\Psi^*(x,t)\Psi(x,t)\,dx$
$\Rightarrow$ probability of finding particle between x and $x + dx$.

iv) Probability should sum to 1. (particle should be somewhere).

$$\int \Psi^*(x,t)\, \Psi(x,t)\, dx = 1$$

In-class 6-4

* Hint: $\sin^2(x) = \frac{1}{2}[1 - \cos(2x)]$

* discuss probability current slide.

* recall: $\Delta f = \nabla^2 f$, $\nabla = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)$

$$\text{\& } \Delta f = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}$$