QUANTUM MECHANICS II : SCHRÖDINGER WAVE EQUATION
THE UNCERTAINTY PRINCIPLE, QM MEASUREMENT, EPR PARADOX

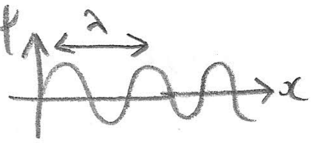
SCHRÖDINGER EQUATION — A recipe for finding an equation for the 'wave characteristic' of a particle e.g an electron. More general than the Bohr model.

de Broglie : $\boxed{\lambda = \frac{h}{p}}$ (λ: wavelength; h: planck's constant; p: momentum)

$$\boxed{\begin{aligned} h &= 6.63\times10^{-34}\,m^2kgs^{-1} \\ \hbar &= h/2\pi \end{aligned}}$$

$\therefore \quad p = \frac{h}{2\pi}\times\frac{2\pi}{\lambda} \quad \therefore \quad \boxed{p = \hbar k}$

$\frac{2\pi}{\lambda}$: wavenumber k



FOURIER SERIES $\Rightarrow$ all waves $\psi(x,t)$ ("Disturbance") can be a sum of sines (or cosines) with different amplitude, frequency, initial phase.

so let $\boxed{\psi(x,t) = Ae^{i(kx-\omega t)}}$ (x: position, t: time)

{ de-Moivre $e^{i\theta} = \cos\theta + i\sin\theta$ so real or imaginary part of $\psi(x,t)$ yields a sinusoid }

$\therefore \quad \boxed{\frac{\partial^2\psi}{\partial x^2} = -k^2\psi}$ $\qquad [\,i^2 = -1\,]$

Now from (classical, nonrelativistic) physics

$$\boxed{\underbrace{\frac{p^2}{2m}}_{KE} + \underbrace{V}_{\text{Potential energy}} = \underbrace{E}_{\text{Total energy}}}$$

$\therefore \quad p^2 = 2m(E-V)$

From $p = \hbar k \Rightarrow p^2 = \hbar^2 k^2$

$\therefore \quad k^2 = p^2/\hbar^2 = \frac{2m(E-V)}{\hbar^2} \quad \therefore \quad \frac{\partial^2\psi}{\partial x^2} = -\frac{2m(E-V)}{\hbar^2}\psi$

$\Rightarrow \quad \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi}$ Time independent Schrödinger equation.

Now $\frac{\partial\psi}{\partial t} = -i\omega\psi$ $\qquad$ Now from planck's equation $E = hf = \frac{h}{2\pi}2\pi f = \hbar\omega$

So $\omega = E/\hbar$ $\therefore$ $\frac{\partial \psi}{\partial t} = -\frac{iE\psi}{\hbar}$

$\Rightarrow$ $\boxed{E\psi = i\hbar \frac{\partial \psi}{\partial t}}$ [$\frac{1}{i} = -i$
ie $i^2 = -1$
$\therefore i = -\frac{1}{i}$]

So Time Dependent Schrödinger equation is: (for particle of mass m)

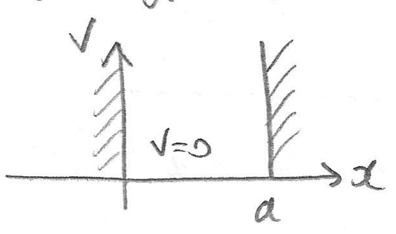
$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t}}$$

What does $\psi(x,t)$ mean? BORN INTERPRETATION

$|\psi(x,t)|^2 dx$ is probability of particle being in location range $x \to x+dx$. CHANCE (UNCERTAINTY) is 'baked into' Quantum mechanics!

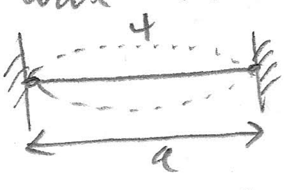
The Simplest (interesting) solution of the Schrödinger Equation is for a particle in a box ie

$$V = \begin{cases} \infty & x \leq 0,\ x \geq a \\ 0 & 0 < x < a \end{cases}$$

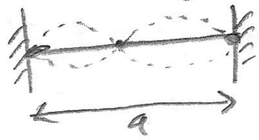


Clearly $\psi = 0$ outside box, and box has symmetry
So let $\boxed{\psi(x,t) = X(x)T(t)}$ and $\boxed{X(x) = A\sin\left(\frac{n\pi x}{a}\right)}$

ie just like a standing wave on a clamped string
(n = integer). ie



or

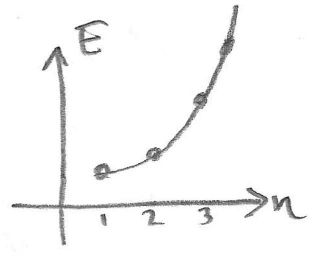


• nodes.

[So $\frac{n\lambda}{2} = a$ and $\psi(x) = A\sin\left(\frac{2\pi x}{\lambda}\right)$ $\therefore$ $\psi(x) = A\sin\left(\frac{n\pi x}{a}\right)$]

$\therefore$ In S.E.: $-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi \longrightarrow -\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2(-1)XT = EXT$

$\Rightarrow$ $\boxed{E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2}$



Now $\quad E X T = i\hbar X \frac{dT}{dt} \qquad \left(E\psi = i\hbar \frac{\partial \psi}{\partial t} \right)$

$$\Rightarrow \quad -iE/\hbar \, dt = \frac{dT}{T}$$

$$\Rightarrow \quad \frac{-iEt}{\hbar} = \ln T + \text{const} \quad \Rightarrow \quad \boxed{T = T_0 e^{-iEt/\hbar}}$$

So absorbing constant T_0 into A

$$\therefore \quad \psi(x,t) = A \sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar} \qquad E_n = \frac{\hbar^2\pi^2}{2ma^2} n^2$$

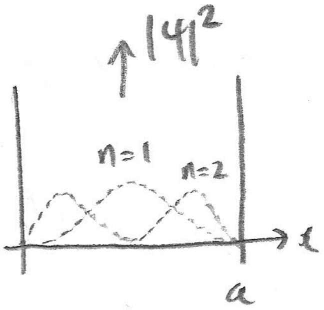
Now from Born: $\boxed{\int_0^a |\psi|^2 dx = 1}$

$|\psi|^2 = \psi\psi^*$
So $e^{-iE_n t/\hbar}$
will become
$e^{-iEt/\hbar} e^{iEt/\hbar} = 1$

$$\therefore \quad A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$A^2/2 \int_0^a \left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) dx = 1$$

$$\Rightarrow \quad \frac{A^2}{2} a = 1 \quad \therefore \quad \boxed{A = \sqrt{\frac{2}{a}}}$$



So
$$\boxed{\begin{aligned} \psi(x,t) &= \sqrt{2/a}\, e^{-iE_n t/\hbar} \sin\left(\frac{n\pi x}{a}\right) \\ E_n &= \frac{\hbar^2\pi^2}{2ma^2} n^2 \end{aligned}}$$

Now standard deviations ("uncertainties")

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} \qquad [\, \langle x^2\rangle - \langle x\rangle^2 \text{ is "variance"} \,]$$

$\boxed{\langle x\rangle = \frac{1}{2}a}$ (obviously from symmetry) $= \int_0^a x|\psi|^2 dx$

$$\langle x^2\rangle = \int_0^a x^2 |\psi|^2 dx = \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx$$

..... lots of algebra ("By Parts" twice ....) $= \frac{1}{3}a^2\left(1 - \frac{3}{2n^2\pi^2}\right)$

$\therefore \quad \Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{1}{\sqrt{12}} a \left(1 - \frac{6}{n^2\pi^2}\right)^{\frac{1}{2}}$

Now $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle}$ Now since box is symmetric expect as much left momentum as right! $\therefore \boxed{\langle p\rangle = 0}$

Now from $\frac{p^2}{2m} + V = E$ and $V=0$ in box

$\Rightarrow \quad p^2 = 2mE. \qquad E = \frac{\hbar^2\pi^2 n^2}{2ma^2}$

$\therefore \quad p^2 = \frac{\hbar^2 \pi^2 n^2}{a^2}$

So for given n, p^2 is a constant $\therefore \langle p^2\rangle = \frac{\hbar^2\pi^2 n^2}{a^2}$

$\therefore \boxed{\Delta p = \frac{\hbar \pi n}{a}}$ Hence $\Delta p \Delta x = \frac{\hbar \pi n}{\sqrt{12}} \left(1 - 6/n^2\pi^2\right)^{\frac{1}{2}}$

$\sqrt{12} = \sqrt{4 \times 3}$
$= 2\sqrt{3}$

$\Rightarrow \quad \Delta p \Delta x = \frac{\hbar}{2}\left(\frac{\pi^2 n^2}{3} - \frac{\pi^2 n^2}{3} \times \frac{6}{n^2\pi^2}\right)^{\frac{1}{2}}$

$\boxed{\Delta p \Delta x = \frac{\hbar}{2}\left(\frac{\pi^2 n^2}{3} - 2\right)^{\frac{1}{2}}}$ when $n=1$: $\sqrt{\pi^2/3 - 2} = \boxed{1.14}$

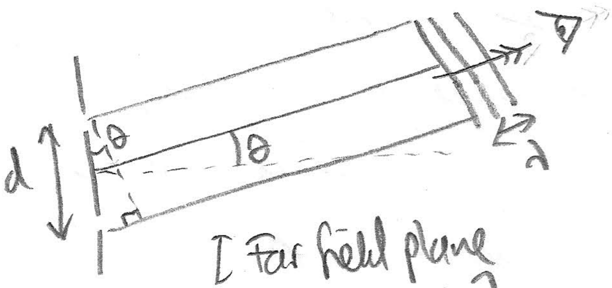
So $\boxed{\Delta p \Delta x > \frac{\hbar}{2}}$ for particle in a box ($\forall n$)

This is an example of the $\boxed{\text{Heisenberg Uncertainty Principle}}$ – a general result.
$\Delta p \Delta x \geq \hbar/2$

Note $\boxed{\Delta E \Delta t \geq \hbar/2}$ is also true.

So you can be more certain about momentum, but at a price of being less certain about position etc.

UNCERTAINTY PRINCIPLE FROM ELECTRON DIFFRACTION

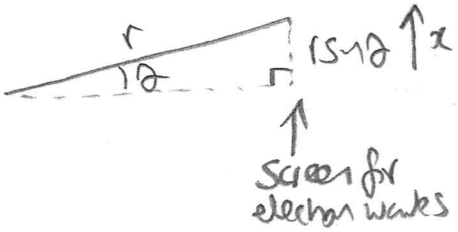


[Far field plane wave approx.]

For constructive interference of electron waves (diffracted by an atomic lattice of spacing d)

$\frac{2\pi}{\lambda} d\sin\theta = 2\pi n$ n integer

$\therefore \boxed{\sin\theta = \frac{n\lambda}{d}}$



Now position of electron wave diffraction pattern rings on a screen is $x = r\sin\theta$.

So imagine a variety of electron waves of wavenumber k

$k = 2\pi/\lambda$ so $\sin\theta = \frac{n}{d} \times \frac{2\pi}{k}$ $\therefore x \propto \frac{1}{k}$

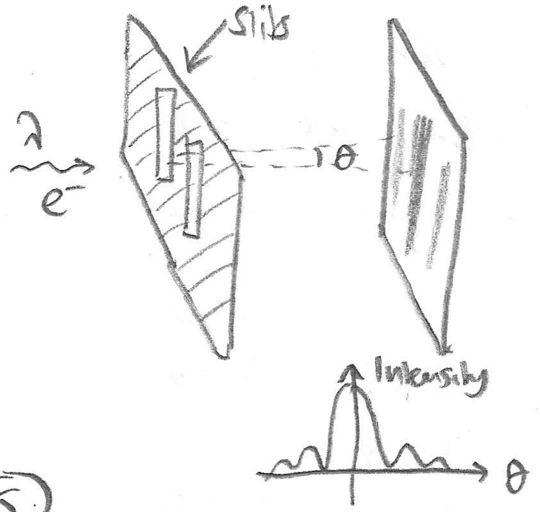
$\therefore$ Expect $\boxed{\Delta x \propto \frac{1}{\Delta k}}$ Now from de-Broglie: $p = \hbar k$

$\therefore \Delta p = \hbar \Delta k$

So expect $\Delta x = \frac{\text{constant} \times \hbar}{\Delta p}$ or $\boxed{\Delta x \Delta p = \hbar \times \text{constant}}$

[which points towards $\Delta p \Delta x \geq \hbar/2$, but not the inequality yet]

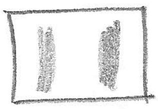
QM & Measurement



The electron wave idea ⇒ you get an $\boxed{\text{interference pattern}}$ if you fire a beam of electrons at a double slit.

But what if you fire one electron at a time?

→ You still get the same pattern ($\propto |\psi|^2$) built up over time!

BUT if you work out which slit the electron passes through you get 

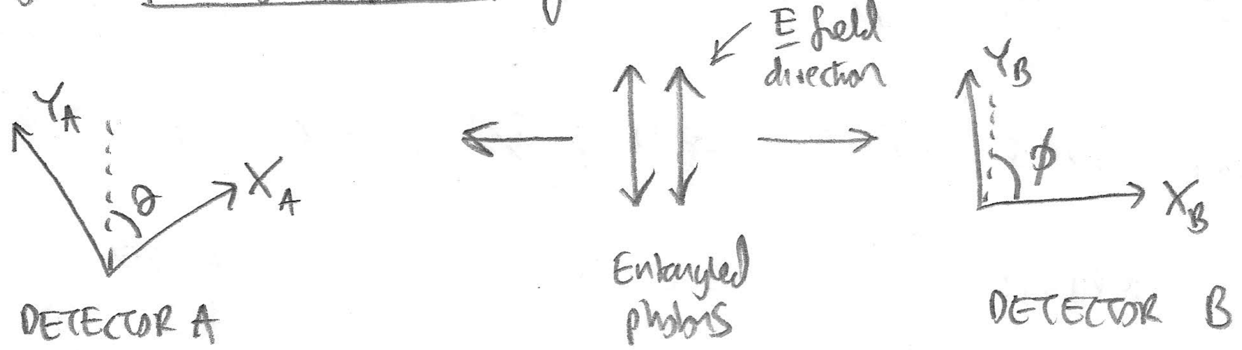
ie PATTERN COLLAPSES.

$\Rightarrow$ Strange paradigm of **Measurement in QM**.

"Copenhagen interpretation". Prior to measurement a WAVEFUNCTION (which represents the state of a system) can be written as a <u>superposition</u> of possible outputs ("eigenstates") of the measurement system. When you make a measurement, THE WAVEFUNCTION COLLAPSES to one of these states. This is the idea of **Schrödinger's Cat** thought experiment.

* Cat in sealed box with poison activated via random radioactive decay.
* Open box, cat is (i) alive or (ii) dead
  Eigenstates are ALIVE or DEAD
* Until box is opened cat is a <u>superposition</u> of BOTH ALIVE and DEAD states (!!)

Another classic example is the **Aspect** experiment (1972) relating to **entangled photons** of the same initial (vertical) polarization



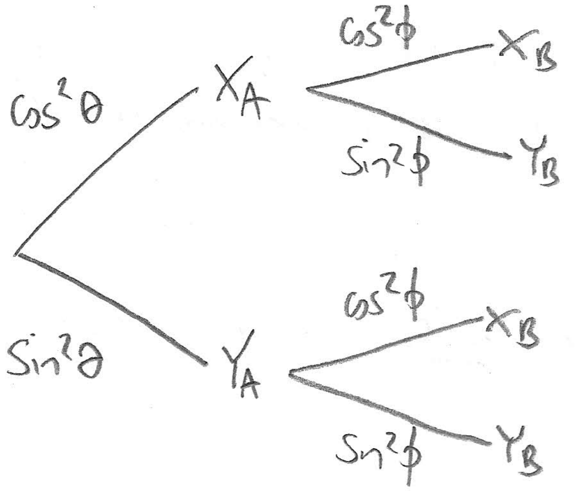
photons (eg from $e^+ + e^- \rightarrow 2\gamma$ annihilation) pass to detectors A, B in opposite directions. The polarization directions X, Y of the detectors is as shown, angles θ, ϕ from vertical.

Expect (Malus' law) probabilities:

[ie we have a long series of photons transmitted so can do stats]

$$P(X_A) = \cos^2\theta$$
$$P(Y_A) = \sin^2\theta$$
$$P(X_B) = \cos^2\phi$$
$$P(Y_B) = \sin^2\phi$$

Classical scenario is measurement of polarization X, Y from detector A to be independent of B

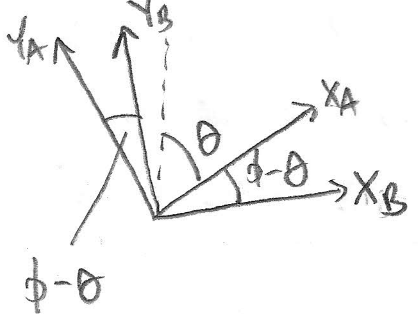


$\therefore$ P(Mismatch)

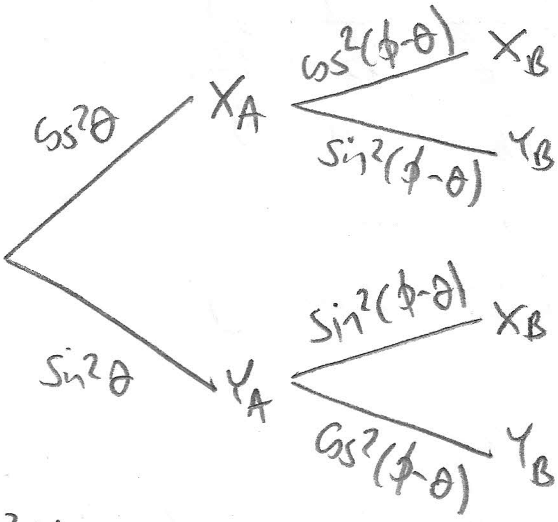
$= P(X_A, Y_B) + P(Y_A, X_B)$

$= \boxed{\cos^2\theta \sin^2\phi + \sin^2\theta \cos^2\phi}$

In QM scenario, if you measure X_A <u>THEN THIS IS WHAT IT BECOMES</u>



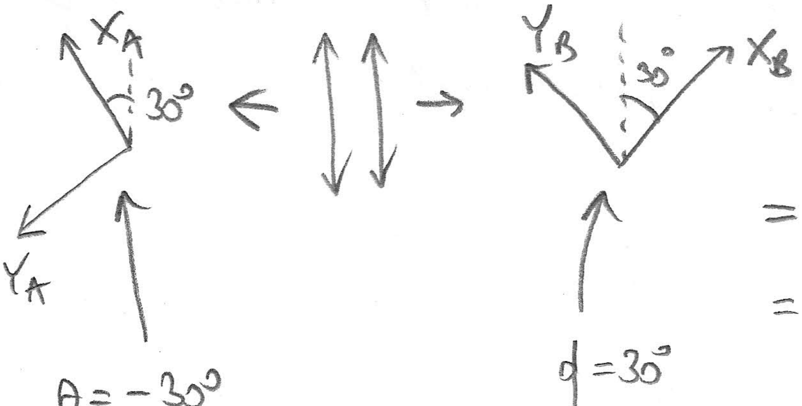
So:

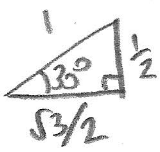


$\therefore$ P(mismatch) $= \cos^2\theta \sin^2(\phi-\theta) + \sin^2\theta \sin^2(\phi-\theta)$

$= \boxed{\sin^2(\phi-\theta)}$ $\quad [\cos^2\theta + \sin^2\theta = 1]$

Example:





$[\cos 30° = \sqrt{3}/2 \quad \sin 30° = \frac{1}{2}]$
$\sin 60° = \sqrt{3}/2$

So classical: P(mismatch)

$= \left(\frac{3}{4}\right)\left(\frac{1}{4}\right) + \left(\frac{1}{4}\right)\left(\frac{3}{4}\right)$

$= \boxed{3/8}$

QUANTUM: P(mismatch)

$= 3/4 = \boxed{6/8}$ ie $\boxed{\text{twice as likely}}$

So what does this mean?
In QM, we measure A first .... and then faster-than-light communication is sent to B? Doesn't this violate Special Relativity? Or are the photons 'as one' and since no time elapses for a photon, then this is ok?

And in terms of measurement - who/what is doing it? What is the mechanism? What <u>Scale</u> does it become important?

Major philosophical, and technical (eg $\boxed{\text{Quantum computing}}$ ** $\boxed{\text{Quantum cryptography}}$ *) applications. A curious idea (Everett 1930-1982) is that "all possible outcomes are realized in parallel universes". Each time a waveform collapses due to 'measurement' a new Universe is created. Personally I <u>REALLY HATE THIS IDEA!</u>

** You are not restricted to 0,1 states. For certain calculations, a quantum computer can be <u>MUCH</u> faster

* If you base a system on the Aspect entangled photons - your X,Y stats should indicate whether an $\boxed{\text{eavesdropper}}$ has intercepted your message.