The Quantum Mechanical Postulates

It was only about 20 years after Planck's bold hypothesis that we finally began to understand QM.

Operationally, the fundamental difference between QM and Classical Mechanics (CM) is that QM can only predict probabilities.

In CM, if one has 100 identical systems, after making a measurement on one of them you can say with certainty that all the other 99 should give the same result, if measured.

In QM identical systems can give different values of the physical quantity being measured, and we can only predict probabilities that various values will be measured.

Let's consider one of the simplest systems and then generalize its features.

The Stern-Gerlach apparatus has a beam of silver atoms passing through an inhomogeneous magnetic field and then being detected on a screen.

Assume that the Ag atom has a magnetic moment $\bar{\mu}$. Then its potential energy in a $\bar{B}$ field is

$$\boxed{U = -\bar{\mu}\cdot\bar{B}} \quad (1)$$

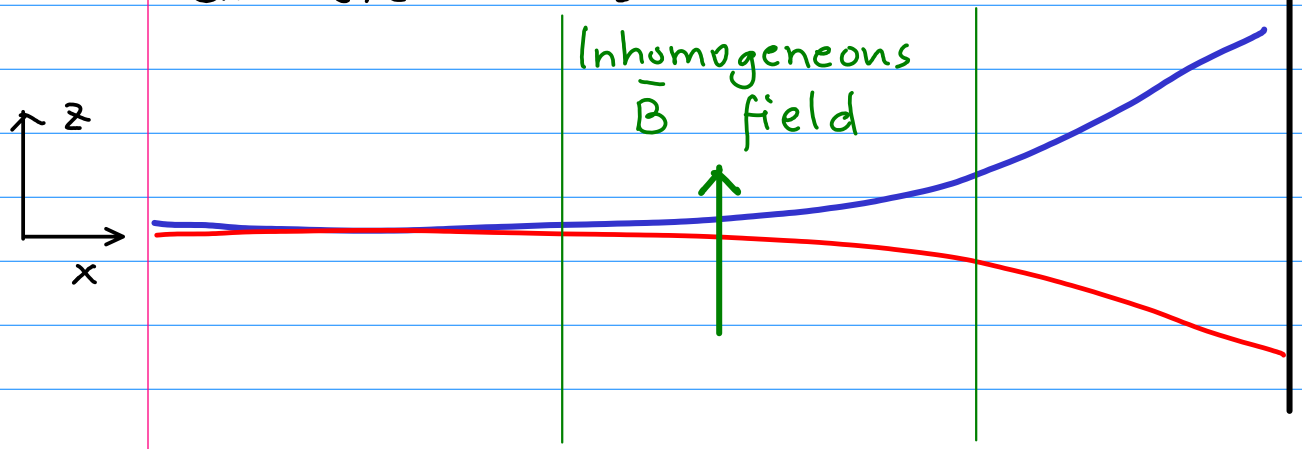
If the field is inhomogeneous, the atoms feel a net force which is the gradient of the potential

$$\boxed{\vec{F} = -\bar{\nabla} U} \quad (2)$$

Atoms with $\bar{\mu}$ aligned with $\bar{B}$ get pushed to regions of stronger field and vice versa. So the atoms suffer a deflection proportional to the component of $\bar{\mu}$ along $\bar{B}$.

Classically, this component is continuous and lies between $-|\vec{\mu}|$ and $+|\vec{\mu}|$.

When the experiment was done in 1922, the deflections observed were only two discrete values.



From later developments, we know that what was being measured was electron spin, and upon measurement it displays only two possible values $\pm\frac{\hbar}{2}$.

Now we can take one of the beams, say the lower one $(-\hbar/2)$ and measure its z-component again. It turns out to remain $-\frac{\hbar}{2}$.

However, if we pass the $-\frac{\hbar}{2}$ beam through another Stern-Gerlach apparatus with the $\bar{B}$ field oriented along y, the beam again splits into two. The values of the measured y-component of $\vec{\mu}$ are again $\pm\hbar/2$.

So far so good. Now we take, say, the upper beam of the y-device and pass it through yet another z-device.

Classically, we would expect to obtain $-\hbar/2$ as the z-component of $\vec{\mu}$. However, the z-device again splits the beam equally between $\pm\hbar/2$.

The y-component measurement has affected the z-component!! The atom seems to have forgotten μ_z after passing through the y-device.

Let us abstract some general features.

First define an ideal measuring device as one that projects the system into one of the possible values of the measured observable (characteristic values = eigenvalues) and leaves the system with a definite value for that observable.

Two different physical observables are said to be compatible if the measurement of one does not affect the measurement of the other

For any system there will be a complete set of compatible measurements. When the results of all these measurements are known, quantum mechanics says this is the most it is possible to know about a system.

In QM we often talk about preparing a system in a pure state. What we mean is that we have measured a complete set of compatible observables and given them definite values.

Identically prepared systems have the same values for all compatible physical observables.

Now we are ready to state the postulates

I) Every pure state corresponds to a ray in a linear space over the complex field known as Hilbert space.
A ray is the (complex) line of kets

$$\boxed{z|\psi\rangle} \quad (3) \qquad z = \text{complex number} \neq 0$$

All elements of a ray are equivalent.

II) Every physical observable is associated with a hermitian operator acting on Hilbert space. The eigenvalues of the operator are the set of allowed values of that observable. If the operator is $\mathbb{M}$ and its eigenvalues are μ_α

$$\boxed{\mathbb{M}\,|\alpha\rangle = \mu_\alpha|\alpha\rangle \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}} \quad (4)$$

then the probability of measuring μ_α in the state $|\psi\rangle$ is

$$\boxed{P(\mu_\alpha) = \frac{|\langle\alpha|\psi\rangle|^2}{|\langle\psi|\psi\rangle|^2}} \quad (5)$$

The Born rule

Furthermore, the state after the measurement is simply $|\alpha\rangle$. This is known as the collapse of the wavefunction and is one of the most counterintuitive postulates.

III) Time evolution is generated by a hermitian operator known as the Hamiltonian, and is given by

$$\boxed{i\hbar \frac{\partial}{\partial t} |\psi\rangle = \mathcal{H} |\psi\rangle} \quad (6)$$

Schrödinger Eq^n

In cases when $\mathcal{H}$ is itself time-independent, it can usually be identified with the energy of the system.

Note that the time-evolution is completely deterministic. All the probabilistic stuff happens when something is measured.

So the counterintuitive aspects have to do with the interaction of a quantum system with a classical measuring device.

However, if QM is really fundamental, one should be able to describe the classical apparatus quantum mechanically.

This intrinsic circularity in the postulates has led to a lot of dissatisfaction, and numerous conceptual frameworks to overcome it.

We will ignore the problem, and just shut up and calculate.

This is all pretty abstract, so let's make it concrete by focusing on the physical observables we know best, x and p in 1 dimension.

For a charged particle it is not too hard to think of good approximations to an ideal detector for $\hat{x}$. One gets the particle to hit a pixel and release a photon, which can be amplified in a photomultiplier tube.

One complication we have to deal with is that the allowed values of x are continuous. We need to generalize the orthonormality to the Dirac delta-f^n

$|x\rangle \equiv$ ket with particle at position x

$\hat{X}$ = operator whose eigenvalue is x

$$\hat{X}|x\rangle = x|x\rangle$$

$$\langle x'|x\rangle = \delta(x-x')$$

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Here is a summary of the definition and properties of the Dirac δ-f^n

$$\boxed{\begin{aligned} \delta(x-x_0) &= \lim_{\sigma\to 0} \frac{1}{\sqrt{\pi}\,\sigma}\, e^{-\frac{(x-x_0)^2}{\sigma^2}} \qquad \text{D1} \\ &= \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(x-x_0)-\eta|k|} \end{aligned}}$$

There are many other representations

$$\boxed{\begin{aligned} \int_{x_1}^{x_2} \delta(x-x_0)\,dx &= 1 \quad \text{if} \quad x_1 < x_0 < x_2 \qquad \text{D2} \\ &= 0 \quad \text{otherwise.} \end{aligned}}$$

$$\boxed{\delta(f(x)) = \sum_{x_i} \frac{\delta(x-x_i)}{|f'(x_i)|} \qquad \text{D3}}$$

where x_i is defined by $f(x_i)=0$

$$\boxed{\begin{aligned} \int_{x_1}^{x_2} dx\, f(x)\,\delta(x-x_0) &= f(x_0) \quad \text{if} \quad x_1 < x_0 < x_2 \\ &= 0 \quad \text{else} \qquad \text{D4} \end{aligned}}$$

$$\boxed{\int_{-\infty}^{\infty} dx\, \delta(x-x_0)\,\delta(x-x_1) = \delta(x_1-x_0) \qquad \text{D5}}$$

Given a ket $|\psi\rangle$ we define its position-space wave function as

$$\boxed{\psi(x) = \langle x|\psi\rangle} \quad (8)$$

So we can rewrite

$$\boxed{|\psi\rangle = \int_{-\infty}^{\infty} dx \; |x\rangle\langle x|\psi\rangle \equiv \int_{-\infty}^{\infty} dx \; |x\rangle \psi(x)} \quad (9)$$

Operator $\hat{x}$

$$\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} dx \; \hat{x}|x\rangle \psi(x)$$

$$\Rightarrow \boxed{\langle x|\hat{x}|\psi\rangle = x\,\psi(x)} \quad (10)$$

The operator $\hat{x}$ acts multiplicatively on the position-space wave function

What kind of linear space are we working in? At the moment we have complex-valued functions of one real variable $-\infty < x < \infty$.

The inner product can be inferred from (9), (7)

$$|\Phi\rangle = \int_{-\infty}^{\infty} dx \; |x\rangle\langle x|\Phi\rangle = \int_{-\infty}^{\infty} dx \; |x\rangle \phi(x)$$

$$\Rightarrow \langle\Phi| = \int_{-\infty}^{\infty} dx \; \phi^*(x)\langle x|$$

$$\boxed{\begin{aligned}\langle \Phi | \Psi \rangle &= \int_{-\infty}^{\infty} dx\ \phi^*(x)\ \langle x| \int_{-\infty}^{\infty} dx'\ |x'\rangle\ \psi(x') \\ &= \int_{-\infty}^{\infty} dx\ \phi^*(x)\,\psi(x)\end{aligned}} \quad (11)$$

The wavefunction of a real physical system has to be normalizable (have finite norm) so we want

$$\boxed{\langle \Psi | \Psi \rangle = \int_{-\infty}^{\infty} dx\ |\psi(x)|^2 < \infty} \quad (12)$$

This is the Hilbert space of square-integrable functions on the real line.

Note that our basis kets $|x\rangle$ do not satisfy this condition! But don't worry, it is OK.

There is another, complementary, basis which is built of eigenstates of momentum.

From de Broglie's hypothesis

$$\boxed{p = h/\lambda = \hbar k} \quad (13) \qquad k = 2\pi/\lambda$$

From classical physics we know that a wave with definite k in 1D looks like

$$\boxed{\text{const}\ e^{ikx}} \quad (14) \quad \text{in real space}$$

So tentatively, we identify a momentum eigenstate as

$$\boxed{\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{ipx}{\hbar}}} \quad (15)$$

From (D1) we see that we should choose the prefactor to be $1/\sqrt{2\pi\hbar}$

$$\boxed{\begin{aligned}\langle p'|p\rangle &= \int_{-\infty}^{\infty} dx\, \langle p'|x\rangle\langle x|p\rangle \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{dx}{\hbar}\, e^{\frac{i}{\hbar}(p-p')x} = \delta(p-p')\end{aligned}} \quad (16)$$

Clearly we can define a momentum operator $\mathbb{P}$ whose eigenstates are $|p\rangle$

$$\boxed{\mathbb{P}|p\rangle = p|p\rangle} \quad (17)$$

Definition of $\mathbb{P}$

Now we can ask, how does $\mathbb{P}$ act in the $|x\rangle$ basis?

What is $\mathbb{P}|x\rangle$?

Since $|p\rangle$ is a complete orthonormal basis we can expand

$$\boxed{|x\rangle = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|x\rangle} \quad (18)$$

or $$\boxed{|x\rangle = \int_{-\infty}^{\infty} dp\ |p\rangle\ e^{\frac{-ipx}{\hbar}}} \quad (19)$$

Now $$\mathbb{p}\,|x\rangle = \int_{-\infty}^{\infty} dp\ \mathbb{p}|p\rangle\ e^{-ipx/\hbar}$$

$$= \int_{-\infty}^{\infty} dp\ p\,|p\rangle\, e^{\frac{-ipx}{\hbar}} = i\hbar \frac{d}{dx}\int_{-\infty}^{\infty} dp\ |p\rangle e^{\frac{-ipx}{\hbar}} = i\hbar \frac{d}{dx}|x\rangle$$

So $$\boxed{\mathbb{p}\,|x\rangle = +i\hbar \frac{d}{dx}|x\rangle} \quad (20)$$

Given this we can ask a further question. How does $\mathbb{p}$ act on a wavefunction in the x-basis?

$$\boxed{\mathbb{p}\,|\psi\rangle = \int_{-\infty}^{\infty} dx\ \mathbb{p}|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\ \psi(x)\ i\hbar\frac{d}{dx}|x\rangle} \quad (21)$$

Integrate by parts, assuming

$$\lim_{|x|\to\infty} \psi(x) = 0$$

$$\Rightarrow \quad \mathbb{p}\,|\psi\rangle = \int_{-\infty}^{\infty} dx\ \left(-i\hbar\frac{d}{dx}\psi(x)\right)\ |x\rangle$$

$$\boxed{\langle x|\mathbb{p}|\psi\rangle = -i\hbar\frac{d}{dx}\langle x|\psi\rangle} \quad (22)$$

We will often abuse notation and simply write

$$\boxed{p\,\psi(x) = -i\hbar \frac{d}{dx}\psi(x)} \quad (23)$$

Let's quickly verify that $\mathbb{P}$ as defined by (21) is a hermitian operator. Recall the hermitian adjoint of $\mathbb{M}$ is defined such that

$$\langle \Phi | \mathbb{M} \Psi \rangle = \langle \mathbb{M}^{+} \Phi | \Psi \rangle$$

or $$\int_{-\infty}^{\infty} dx\, \langle \Phi | x \rangle \langle x | \mathbb{M} | \Psi \rangle = \int_{-\infty}^{\infty} dx\, \langle \mathbb{M}^{+} \Phi | x \rangle \langle x | \Psi \rangle$$

$$LHS = \int_{-\infty}^{\infty} dx\, \Phi^{*}(x) \left(-i\hbar \frac{d}{dx} \Psi(x) \right)$$

Integrate by parts, assuming

$$\lim_{|x| \to \infty} \Psi(x), \Phi(x) = 0$$

$$LHS = \int_{-\infty}^{\infty} dx \left(+i\hbar \frac{d}{dx} \Phi^{*}(x) \right) \Psi(x)$$

$$= \int_{-\infty}^{\infty} dx \left(-i\hbar \frac{d}{dx} \Phi(x) \right)^{*} \Psi(x)$$

$\Rightarrow$ $-i\hbar \frac{d}{dx}$ is to be identified with $p^\dagger$

So $\boxed{p^\dagger = p}$ (24) p is hermitian

Now we are ready to talk about the (in) compatibility of measuring x and p.

Here is a general result: If two linear operators A and B commute, they share the same eigenvectors and are compatible.

We define the commutator of A and B as

$$\boxed{[A, B] = AB - BA} \quad (25)$$

Suppose $\boxed{[A, B] = 0}$ (26) and A has eigenvectors $|\alpha\rangle$ with eigenvalues a_α

$$\boxed{A|\alpha\rangle = a_\alpha|\alpha\rangle} \quad (27)$$

Consider

Use (26)

$$\boxed{A(B|\alpha\rangle) = (AB)|\alpha\rangle = BA|\alpha\rangle = a_\alpha B|\alpha\rangle} \quad (28)$$

So $B|\alpha\rangle$ is also an eigenvector of A with eigenvalue a_α. It could happen that the eigenvalue a_α is degenerate, with many eigenvectors corresponding to the same eigenvalue.

Let's first focus on the simpler case, where all the eigenvalues of $\mathbb{A}$ are nondegenerate.

This means $|\alpha\rangle$ has to be an eigenvector of $\mathbb{B}$ also

$$\boxed{\mathbb{B}|\alpha\rangle = b_\alpha |\alpha\rangle} \quad (29)$$

If a_α is degenerate $\mathbb{B}$ must act within the degenerate subspace. Then diagonalize $\mathbb{B}$ in the degenerate subspace to show that $\mathbb{A}$ and $\mathbb{B}$ share all their eigenvectors.

Consider the following thought experiment.

We pass the system first through an apparatus that measures the physical observable $\mathbb{A}$, selecting the particular eigenstate $|\alpha\rangle$

If $[\mathbb{A}, \mathbb{B}] = 0$, $\mathbb{A}$ and $\mathbb{B}$ are compatible and $\mathbb{B}$ will give a definite result on $|\alpha\rangle$ (b_α) upon measurement, and leave $|\alpha\rangle$ undisturbed

If $[\mathbb{A}, \mathbb{B}] \neq 0$ then the observables $\mathbb{A}$ & $\mathbb{B}$ are incompatible, and in general $\mathbb{B}$ when measured in $|\alpha\rangle$, it will not give a definite result, and will generically change $|\alpha\rangle$.

The extreme case of incompatibility is given by the operators $\mathbb{x}$ and $\mathbb{p}$.

On any wave f^n $\psi(x) \equiv \langle x|\psi\rangle$

$$(\mathbb{x}\psi)(x) = x\,\psi(x)$$
$$(\mathbb{p}\psi)(x) = -i\hbar \frac{d}{dx}\psi(x)$$

$$\boxed{\begin{aligned}([\mathbb{x},\mathbb{p}]\psi)(x) &= -i\hbar\left\{x\frac{d}{dx}\psi(x) - \frac{d}{dx}(x\,\psi(x))\right\} \\ &= i\hbar\,\psi(x)\end{aligned}} \quad (30)$$

Since this is true for any $\psi(x)$

$$\boxed{[\mathbb{x},\mathbb{p}] = i\hbar\,\mathbb{1}} \quad (31)$$

This is the canonical commutation relation.

The most important consequence of this is Heisenberg's Uncertainty principle, which we will cover a few weeks from now.

Let us briefly consider interference. First we will look at light.

As you all know light of a given wavevector $\vec{k}$ can have two independent polarizations satisfying

$$\boxed{\hat{\epsilon}\cdot\vec{k} = 0} \quad (32)$$

$\hat{\epsilon}$ = polarization direction

We can define two perpendicular polarization directions

$$\boxed{\hat{\epsilon}_1 \cdot \bar{k} = \hat{\epsilon}_2 \cdot \bar{k} = 0 \qquad \hat{\epsilon}_1 \cdot \hat{\epsilon}_2 = 0} \quad (33)$$

A coherent plane wave can be written as

$$\boxed{\vec{E}(\bar{x},t) = \operatorname{Re}\left\{ \left(\mathcal{E}_{01}\hat{\epsilon}_1 + \mathcal{E}_{02}\hat{\epsilon}_2 \right) e^{i(\bar{k}\cdot\bar{x} - \omega t)} \right\}} \quad (34)$$

where $\mathcal{E}_{01}$ and $\mathcal{E}_{02}$ are complex numbers.

$$\boxed{\mathcal{E}_{01} = |\mathcal{E}_{01}| e^{i\varphi_1} \qquad \mathcal{E}_{02} = |\mathcal{E}_{02}| e^{i\varphi_2}} \quad (35)$$

If $\varphi_1 = \varphi_2$ or $\varphi_2 + \pi$ (or if one of $|\mathcal{E}_{01}|$ or $|\mathcal{E}_{02}| = 0$) the wave is linearly polarized

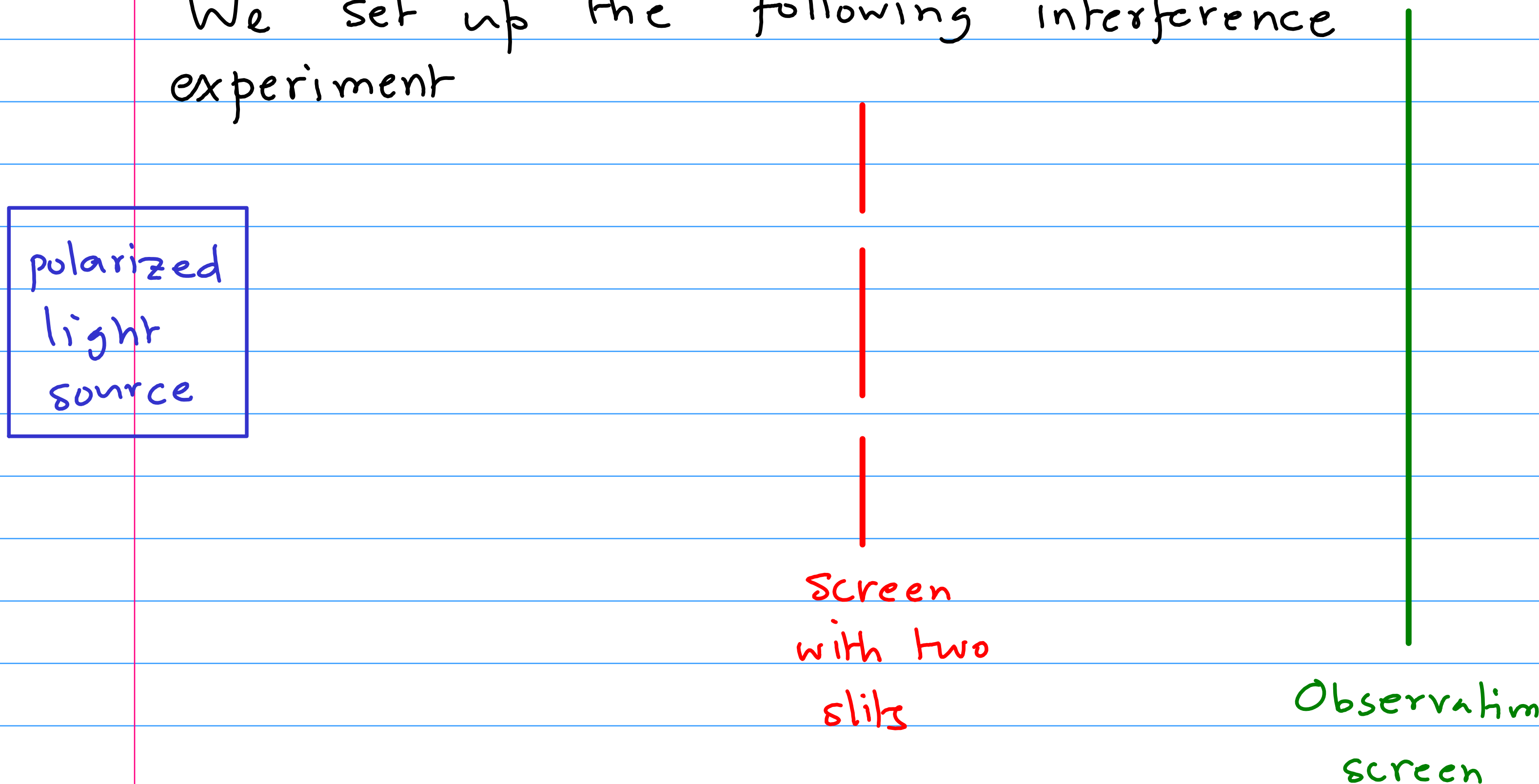
For generic values of $\mathcal{E}_{01}, \mathcal{E}_{02}$ the wave is elliptically polarized.

There are crystals called polarizers that allow only one (linear) polarization, so one can prepare a wave in a definite state of linear polarization.

Classically, light is an EM wave, so it undergoes interference. However, light also behaves like a particle when it interacts with electrons.

To smoothly go from one to the other

We set up the following interference experiment



Initially we send a high intensity wave and observe classical interference. We explain this by saying that different parts of the wave go via the two slits and recombine at the observation screen.

Now we decrease the intensity of the source till it emits one photon at a time. At the screen each photon hits at a definite spot, because the electrons in the pixels can only absorb the full $\hbar\omega$. The spot where the photon will hit cannot be predicted.

As the photons keep coming they build up the interference pattern.

If one thinks of a photon as a classical particle following a trajectory this seems impossible to explain.

Quantum mechanically, we understand this as an instance of complementarity where the photon acts like a wave when going through the slits but acts like a particle when being absorbed by the electron.

If one tries to find out which path the photon took, by, say, putting a photon detector near one slit, this destroys the interference.

All the statements made above for photons are true of microscopic particles as well. They too behave like waves when going through the slits, but like particles when they are detected.

One can do an even simpler experiment with photons. For convenience let us assume that $\bar{k}$ is pointing out of the page. We will call this the $\hat{z}$ direction

We first prepare a wave with polarization along $\hat{x}$, and then we put in its path a polarization filter oriented along

$$\boxed{\hat{n} = \hat{x}\cos\theta + \hat{y}\sin\theta} \quad (36)$$

Classically, it is clear what to do. We started with an x-polarized beam

$$\boxed{\vec{E} = \hat{x} E_0 e^{i(kz-\omega t)}} \quad (37)$$

We decompose this into a field along $\hat{n}$ and one $\perp$ to $\hat{n}$

$$\boxed{\hat{x} = \hat{n} \cos\theta - (\hat{z} \times \hat{n}) \sin\theta} \quad (38)$$

Only the component along $\hat{n}$ gets through the filter. So the intensity of the final beam is

$$\boxed{E_0^2 \cos^2\theta} \quad (39)$$

Once again we reduce the intensity of the wave till only one photon at a time goes through the apparatus.

Now we find that each time a photon hits the $\hat{n}$-filter it either gets through or not. This is impossible to predict for each photon. However, after many many photons have hit the filter we find that a fraction $\cos^2\theta$ of them got through. This is another instance of complementarity.

So far we have not said much about the Hamiltonian. This will be the topic of the next set of notes