accelerated charges are the sources of (electromagnetic) radiation.

What is wrong with both Newtonian Mechanics and Classical Electrodynamics?

By the end of the XIX century there was mounting experimental evidence of difficulty with this picture.

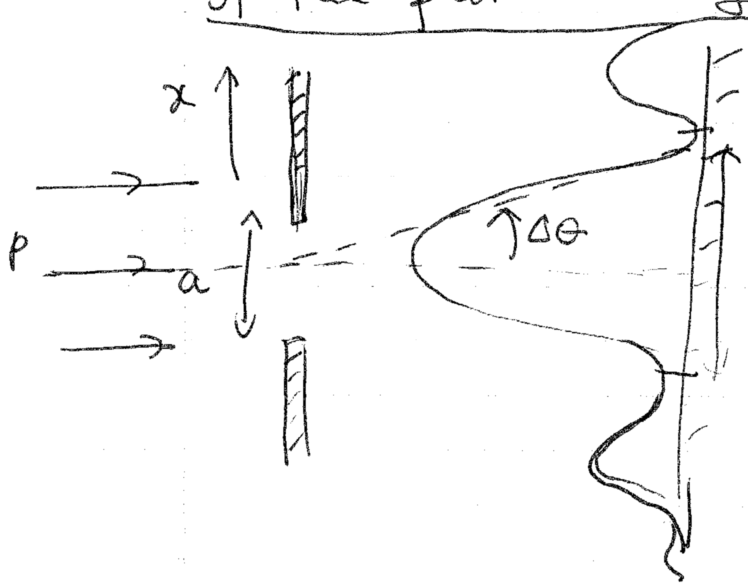
1) There was evidence that light can act as a set of particles, photons. This was first recognized in the spectrum of blackbody radiation which was consistent with the hypothesis that the energy of a monochromatic wave of frequency ν was quantized

$E = h\nu = \hbar\omega \qquad \hbar = h/2\pi$

$h = 6.3 \times 10^{-27}$ erg sec Planck's constant.

Later on Einstein explained successfully the photoelectric effect by assuming that a light wave is a collections of photons each carrying energy $E = h\nu$ and momentum $p = \frac{h}{\lambda} = \hbar k$ (Compton). In other terms under some circumstances light behaved as a collection of *particles*.

(L8) How about the evidence for wave behavior, such as diffraction? Subsequent experiments showed that the diffraction pattern is formed by the impact of *individual* photons acting very much *like particles*. In other terms light has a *dual* nature: some of the times it acts as a wave and some of the times as a particle. It is important to keep in mind that it behaves like a particle when the *position* of the photon *is measured* (as in the film when the diffraction pattern is recorded) while it behaves like a *wave* in the way it propagates in space, i.e. the origin of the diffraction pattern itself. Hence if we use a slits of aperture a to measure the position of the photon along the x axis, the width of



the diffraction peak is

$$\Delta\theta = \frac{\lambda}{a}$$

and the spread of momentum on the x axis is

$$\Delta p_x = p\,\Delta\theta = p\frac{\lambda}{a}$$

But $p = \frac{h}{\lambda} \Rightarrow \lambda p = h$ and $\Delta x = a$

$$\Rightarrow \boxed{\Delta x\,\Delta p_x \sim h}$$

This is an example of an uncertainty relation. What does it mean? If the diffraction experiment is done with a low intensity light source Classically (i.e. from Maxwell's Eqns.) we would have predicted ~~that~~ That simply the overall intensity of the diffraction pattern will be proportionally reduced. However experimentally it is found that the diffraction pattern is formed by the impact of individual photons which over time reproduce the diffraction pattern. In other terms the diffraction pattern can be interpreted as a histogram, i.e. as the $\boxed{\text{probability}}$ that a photon will be absorbed at a given location on the screen. Thus the quantization of the electromagnetic field led us to a probabilistic interpretation of the diffraction experiment. From this point of view Δx is the uncertainty of the measurement of the position of the photon (~~as~~ measured by the ~~[illegible]~~ slit) while Δp_x is the uncertainty in the momentum along the screen (the x axis). The uncertainty relation means that any attempt at defining the position with more precision ($\Delta x \to 0$) will necessarily increase the uncertainty of the measurement of its momentum $\Delta p_x \sim \frac{h}{\Delta x} \to \infty$

From Maxwell's Equations, and from the wave equation which follows from it, we know that an electromagnetic wave has the form

$$\vec{A}(\vec{x},t) = \vec{A}_0 \; e^{i(\vec{k}.\vec{x} - \omega t)} \qquad \omega = |\vec{k}|c$$

Notice that since $\vec{\nabla}.\vec{A} = 0 \Rightarrow \vec{k}.\vec{A}_0 = 0$

$\Rightarrow$ $\vec{A}_0$ is a vector $\perp$ $\vec{k}$. Given $\vec{k}$ there are $\underline{\underline{2}}$ perpendicular directions, i.e. two polarizations $\hat{e}_1(\vec{k})$ and $\hat{e}_2(\vec{k})$ / $\hat{e}_i(\vec{k}) \cdot \hat{e}_j(\vec{k}) = \delta_{ij}$

$$\hat{e}_i(\vec{k}) \, . \, \vec{k} = 0$$

$$\Rightarrow \vec{A}_j(\vec{x},t) = A_0 \; \hat{e}_j(\vec{k}) \; e^{i(\vec{k}.\vec{x} - \omega t)}$$

$$\Rightarrow \begin{cases} \vec{E}(\vec{x},t) = -\dfrac{1}{c}\dfrac{\partial \vec{A}}{\partial t} = \dfrac{i\omega}{c} \vec{A}_j \\ \\ \vec{B}(\vec{x},t) = \vec{\nabla} \times \vec{A} = i\vec{k} \times \vec{A}_j \end{cases}$$

whereas the energy density is

$$\mathcal{E} = \frac{1}{2}\left(\vec{E}^2 + \vec{B}^2\right) = \frac{1}{2}\left(\frac{\omega^2}{c^2} + \vec{k}^2\right)\vec{A}^2 = \frac{\omega^2 \vec{A}^2}{c^2}$$

$\Rightarrow$ the energy density $\propto \vec{A}^2$ (or rather $\vec{E}^2$)

However, classical waves (e.g. e.m. waves) obey a <u>superposition principle</u> $\Rightarrow$ the total intensity at a given point $(\vec{x}, t)$ is <u>not</u> the sum of the intensities but the square of the sum of the amplitude. This is so because the wave equation (i.e. Maxwell's Equation) is <u>linear</u>. This leads to the phenomenon of <u>interference</u> which is a consequence of the fact that the phase difference between two waves cannot be changed once it is fixed ⇒ phase coherence.

However we just concluded that the intensity of the diffraction pattern, ~~and~~ hence also of the interference patterns as well, tells us the <u>probability</u> of finding a <u>photon</u> at $\vec{x}$ at some time t. Thus the important physical quantity is the <u>amplitude</u> whose square (absolute value square) is the probability.

<u>Quantization and Energy Levels</u>

We just saw that we ~~were~~ are forced to take the point of view that the electromagnetic field is actually quantized ⇒ it is decomposed into a set of photons, particle-like objects with energy $E = \hbar\omega = h\nu$ ~~and~~, momentum $\vec{p} = \hbar\vec{k}$ (where $\vec{k}$ is the wave vector) and polarization $\hat{e}_1$ or $\hat{e}_2$ (these are linearly polarized photons; we can also construct RCP and LCP photons in the usual manner). We will show (next semester, in Phys. 481) that the total energy is $N\hbar\omega$ (something that will accept for now).

Let us discuss another consequence of quantization. The fact that ~~since~~ electromagnetic waves can only be ~~created~~ emitted or absorbed (i.e. by charged particles) in quanta implies that something similar must happen to matter as well. Bohr when studying the structure of the atom, assumed in fact that an electron circling around an atom can only be in certain _discrete_ orbits with fixed discrete energies (energy levels) such that the energy differences equal the energy of a photon that is either emitted or absorbed. Photons also carry an _angular momentum_ determined by their helicity which for RCP photons is $\hbar$ whereas for LCP photons is $-\hbar$; Bohr concluded that ~~for~~ if angular momentum is conserved $\Rightarrow$ the <u>angular momentum of the electron</u> itself ~~is~~ also must be quantized.

$\Rightarrow$ the "allowed orbits" must satisfy

$P_\theta = n\hbar$, where $P_\theta = L_z$ is the angular momentum $\perp$ to the plane of the orbit. From this assumption Bohr was able to "derive" a scheme of energy levels which was consistent with the Balmer spectrum of the hydrogen atom.

However, this solution posed more problems than it actually solved, such as ~~Since~~ : why is the ~~too~~ angular momentum quantized ? This is a violation of the rules of Newtonian mechanics. In addition ~~there~~ there was still the problem of the stability of the atom, e.g. why don't electrons radiate when they are in an "energy level"? In addition, Bohr's construction required that the orbits be closed, something that happens only for a $1/r$ potential ~~but~~ and only for a two-body problem. Real atoms have many electrons and ~~#~~ these rules should apply to any potential. So these rules were indicative and suggestive but they were ad-hoc.

A first step in the construction of a "new mechanics" was made by Louis de Broglie who proposed that the electron has a dual nature, partly a wave, partly a particle. DeBroglie proposed that the wavelength of the "pilot wave" λ was $\frac{h}{|p|}$ and that the allowed orbits were such that the waves interfered constructively, as in a resonance. Thus, ~~in~~ a circular orbit of radius R has ~~perimeter~~ circumference $2\pi R = n\lambda$.

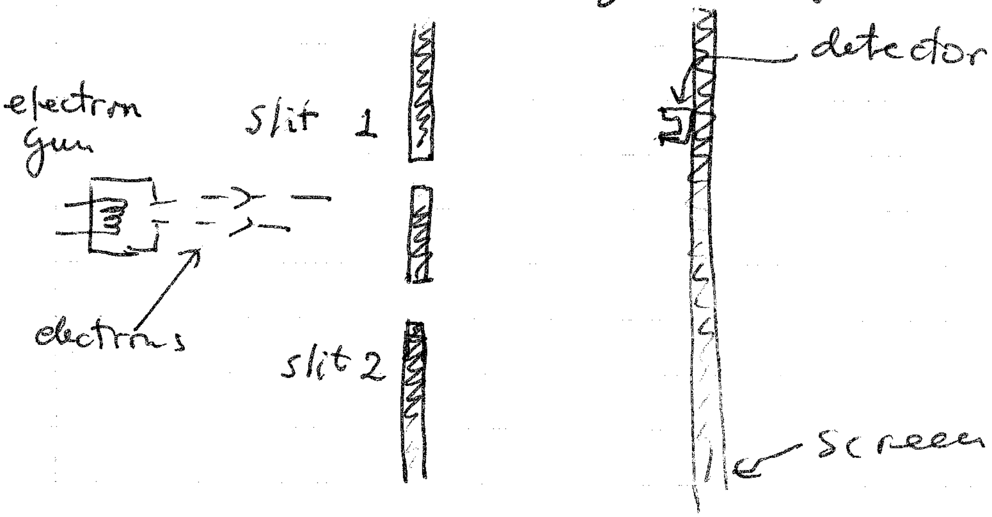
The angular momentum $p_\theta = mvR = pR = \frac{h}{\lambda}\frac{n\lambda}{2\pi}$

$\Rightarrow P_\theta = n\hbar \Rightarrow$ the quantization of P_θ suggests that the electron behaves as a wave.

Thus, according to de Broglie, <u>all matter</u> has a dual particle-wave nature. This idea suggested that an analog of the two-slit interference experiment should also ~~happen to~~ work for electrons as well. However due to the size of the mass of the electron its wavelength (for typical momenta) is so short that it is hard to do this experiment with slits. But it is possible to use a <u>crystal</u> instead, an experiment done ~ 1930 by Davisson and Germer. The result was completely analogous to what is seen ~~f~~ in photons (by now this expt. have also been done with atoms).

How can we understand this effect?

In classical physics, electrons (or any other particle) have well defined trajectories. Thus electrons are in one and only one place at one time. Imagine a thought experiment (a "Gedanken-experiment" in German) in which a collimated beam of electrons is produced (by an electron gun) and sent to hit a "screen" with 2 slits (actually a crystal).



The slits and screens are assumed to be macroscopically large and rigid, and at rest. What do we expect to happen classically? Classical physics will say that at a given point on the screen we detect an electron and that this particle arrived there *either* through slit 1 *or* through slit 2. Consequently if P_1 is the probability ~~distribution~~ to detect a particle at $\vec{x}$ that came through slit 1 and P_2 is the probability that a particle that went through slit 2 also arrives at $\vec{x}$, $\Rightarrow$ the total probability is $P_{12} = P_1 + P_2$ since the particle must go either through 1 or through 2. $\Rightarrow$ In classical physics we add probabilities and this rule is a consequence of the fact that particles have well defined trajectories.

But the experiment shows something very different. It shows an *interference* pattern which is for all practical purposes identical to that of light waves or any other wave-like phenomena. In particular it shows that, instead of adding probabilities (i.e. the # of particles detected over some time τ) we must associate a (complex) *amplitude* to the behavior of the particle and that what is additive are the amplitudes. Like in the case of light waves the absolute value square of the total amplitude at $\vec{x}$ determines the probability.

Notice that the electrons are still detected at $\vec{x}$ as particles, objects that arrive as a whole ~~wit~~ always with the same mass and charge, and with a definite momentum and energy. However, in spite of that, there are places on the screen where no electrons are detected at all (nodes of the interference pattern) whereas at the center the detection rate (the probability) is larger than in the classical prediction. So if we call ϕ_1 the amplitude due to electrons arriving at $\vec{x}$ through slit 1, and ϕ_2 the amplitude ~~of~~ for electrons arriving at $\vec{x}$ through slit 2, the total amplitude is $\phi_1 + \phi_2$ and the probability of detection is

$$P_{12} = |\phi_1|^2 + |\phi_2|^2 + \phi_1^*\phi_2 + \phi_2^*\phi_1$$

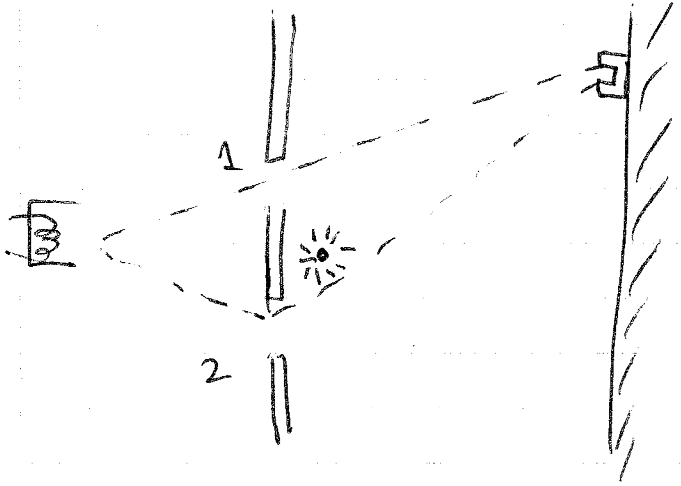
$$\equiv P_1 + P_2 + 2\sqrt{P_1 P_2}\,\cos\delta$$

δ: phase difference. $\Rightarrow P_{12} \neq P_1 + P_2$

$\Rightarrow$ it is not true that the electrons goes through either ~~th~~ slit 1 or slit 2 .

Q: Can we determine experimentally through which slit did the electron go through ?

Let us modify our experiment by adding a light source behind the slits and observe the effects of the electron~~s~~ being scattered by light.



We now that charged ~~part~~ particles scatter light ⇒ as the electron passes through a slit it will scatter light (which we observe) and we can also detect the (scattered) electron at the back screen.

⇒ If the electron goes through 1 ⇒ flash close to 1

if the electron~~s~~ goes through 2 ⇒ flash close to 2 .

what ~~does~~ really happen? Every time an electron is detected (at the back screen) we see a flash either close to 1 or close to 2 .

This would imply that we could in fact determine whether the electron goes through 1 or through 2. But what about the interference pattern observed at the back screen? We can now count the electrons ~~arriving~~ arriving at $\vec{x}$ and keep track through which slit they went through (using the flashes). However now the pattern is the ~~one~~ we would have observed by blocking one slit at a time and just adding them up $\Rightarrow P'_{12} = P_1 + P_2$ $\Rightarrow$ i.e. if we observe through which slit did the electron go through (i.e. we measured it's position) we spoiled the phase coherence & and no interference is observed! $\Rightarrow$ What we obtain depends on whether we look at the electrons or we don't look at them! In particular if we do not look at them we get interference.

~~Wel~~ Well, this means that if we try to measure precisely their position we cannot predict where they will show up (i.e. their momentum).

Suppose we try the same expt. but with photons of longer and longer wavelength. If their wavelength is short compared to the distance d ~~bet~~ between the slits we are in the same situation as before but if $\lambda \gg d$ $\Rightarrow$ due to the wave nature of light we cannot resolve the slits any more and we won't be able to tell through which slot did the electron which scattered the photon actually went through!

Based on these observation Heisenberg proposed his Uncertainty ~~P~~ Principle which at the level of this thought expt. means that it is not possible to design an experiment that will determine the trajectory of the ④ electron without disturbing the interference pattern.

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We conclude with ~~two~~ ~~all three~~ the Principles of Quantum Mechanics

① The behavior of a particle is determined by a complex amplitude whose absolute value squared yields the probability of observing the particle at $\vec{x}$. We will refer to the amplitude as to the state vector or simply as to the "state". Amplitudes will be assumed to form a vector space.

In particular (1.a) If an event can occur in more than one way we must add the amplitudes (Superposition Principle)

② If an experiment ~~possible~~ capable of telling which of the alternatives takes place ⇒ probabilities are added (no interference)

③ ~~If a certain physical quantity of the electron, such as its position, is measured~~
If we measure the position of the electron →

with uncertainty Δx, and we could determine the momentum p_x with uncertainty Δp_x ⇒

$$\Delta x \, \Delta p_x \gtrsim h$$

(Heisenberg's Uncertainty Principle).

④ Physical observables are identified with linear operators acting on the vector space of states. A measurement of an observable is a process by which a state is projected onto an eigenstate of this observable, with the eigenvalue being the result of the measurement. The restriction that the e.v.'s ~~be~~ are real numbers requires that the operators must be Hermitian. This process of projection is usually referred to as "the collapse of the wave function".

⑤ Physical Observables whose operators commute with each other can be measured simultaneously with arbitrary precision and the result of such a measure

-ment ~~is~~ ~~these~~ are their eigenvalues. Such physical observables are said to be compatible. It is generally assumed that ~~there exist~~ for every physical system there exists a complete set of (compatible) commuting observables whose knowledge yields the maximum possible description of the physical system in Quantum Mechanics.

In contrast, observables whose operators do not commute with each other are said to be incompatible. A special but important case are operators whose (non-vanishing) commutator is a complex number (i.e. it is proportional to the identity). These observables are said to be complementary. Complementary observables ~~can be shown to~~ will be shown to obey an Uncertainty Principle (Bohr's Complementarity Principle)

Bohr's Complementarity Principle asserts that dynamical variables ~~[illegible]~~ which are canonically conjugate to each other (in the Hamiltonian sense of Classical Mechanics) cannot be measured simultaneously in QM, and must obey ~~an~~ the Uncertainty Principle.

⑥ The Correspondence Principle

Bohr required the pple. that in situations where Classical Mechanics applies, Quantum Mechanics should reduce to Classical Mechanics. In other terms if a quantum mechanical prediction for some ~~[illegible]~~ observable contains ħ, the result should reduce to the Classical one if ħ → 0. (Go to Math)

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back here

Position and Momentum

Let us begin with the simplest mechanical observables, position and momentum. The principles that we enunciated above state that in QM to each ~~these~~ ~~be~~ observable we must associate a Hermitian operator. Let us

Consider first the case of "a particle in one-dimension". Let $\hat{X}$ be the position operator and $\hat{p}$ the momentum operator. Let $|x\rangle$ be a state in which the particle is localized at x , $\hat{X}|x\rangle = x\,|x\rangle$

Here we have used that to measure a physical quantity is to project the state onto an eigenstate of the observable, in this case $\hat{X}$. Likewise $|p\rangle$ will denote ~~an~~ a state with momentum p and it is an eigenstate of the linear operator $\hat{p}$ with ~~[illegible]~~ eigenvalue p.

In classical mechanics we saw that p and x are canonically conjugate quantities, in the sense that their Poisson Bracket is

$$\{x, p\} = 1$$

~~[illegible]~~ We ~~will~~ associated x and p to the linear operators $\hat{X}$ and $\hat{p}$. What is the meaning of this equation in QM? ~~For begin~~

The Complementarity Principle tells us that these physical observables must obey an Uncertainty Principle and the Correspondence Pple. says that as $\hbar \to 0$ we must recover CM (i.e. a Poisson Bracket). Then, we are led to the statement that

$$\{x, p\} = 1 \longrightarrow [\hat{X}, \hat{P}] \sim I$$

where $\hat{I}$ is the identity operator. Since $\hat{x}^\dagger = \hat{x}$ and $\hat{p}^\dagger = \hat{p}$ (and $\hat{I}^\dagger = I$) we need a constant in front of $I \propto i$. Also since as $\hbar \to 0$ we must be able to do the ~~measure~~ measurement without interference, the constant must $\to 0$ if $\hbar \to 0 \Longrightarrow$

Canonical Quantization Rule:

$$[\hat{x}, \hat{p}] = i\hbar \hat{I} \qquad (\ \hat{I} \text{ will be dropped})$$

We discussed before that the matrix elements of $\hat{x}$ are $\langle x | \hat{x} | x' \rangle = x\, \delta(x - x')$

and we saw that there is an operator ~~$\hat{p}$~~ $-i\hat{D}$

$$\langle x | -i\hat{D} | x' \rangle = -i \frac{d}{dx} \delta(x-x')$$

we also showed that $[\hat{X}, -i\hat{D}] = i \hat{I}$

$\Rightarrow$ we define ~~the~~ a momentum operator $\hat{p}$ such that its matrix elements are

$$\langle x | \hat{p} | x' \rangle = -i\hbar \frac{d}{dx} \delta(x-x')$$

$$\Rightarrow \quad [\hat{X}, \hat{P}] = i\hbar \hat{I} \qquad (\hat{I} = 1)$$

Let us show that these observables obey ~~the~~ the uncertainty principle. To do this we need to consider some state $|\psi\rangle$ which in position space is the "wave function" $\psi(x)$

$$\psi(x) = \langle x | \psi \rangle$$

Let us Fourier expand this function

$$\psi(x) = \int_{-\infty}^{+\infty} \frac{dk}{\sqrt{2\pi}} \; \psi(k) \, e^{ikx}$$

(or $|\psi\rangle = \int dk \; \psi(k) \; |k\rangle$)

We will assume that as $x \to \pm\infty$ $\psi(x)$ obeys self-adjoint boundary conditions.

According to our Principles, $|\psi(x)|^2$ is the normalized probability density to find the particle at x. $\Rightarrow$

$$\langle x\rangle = \int_{-\infty}^{+\infty} dx \quad x \quad |\psi(x)|^2 = \int_{-\infty}^{+\infty} dx \; \langle\psi|x\rangle x \langle x|\psi\rangle$$

$$\equiv \langle\psi|\hat{x}|\psi\rangle$$

check: $$|\psi\rangle = \int dx \; |x\rangle \; \langle x|\psi\rangle$$

$$= \int dx \; \psi(x) \; |x\rangle$$

$$\Rightarrow \quad \langle\psi|\hat{x}|\psi\rangle = \int dx \int dx' \; \langle x|\hat{x}|x'\rangle \psi^*(x)\psi(x')$$

$$= \int dx \int dx' \; x \, \delta(x-x') \; \psi^*(x) \; \psi(x')$$

$$= \int dx \quad x \, |\psi(x)|^2 \qquad \checkmark$$

What is the variance$^{\Delta x}$ of the measurement of the position?

$$(\Delta x)^2 \equiv \langle(\hat{x} - \langle x\rangle)^2\rangle$$

$$= \langle\psi|(\hat{x} - \langle x\rangle)^2|\psi\rangle$$

$$= \langle\psi|\hat{x}^2|\psi\rangle - \langle\psi|\hat{x}|\psi\rangle^2$$

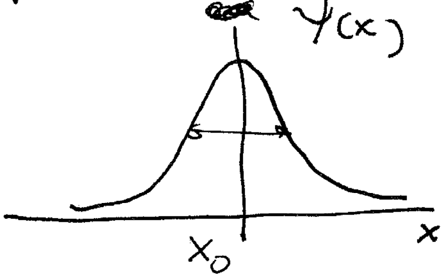
$$= \int_{-\infty}^{+\infty} dx \; x^2 \, |\psi(x)|^2 - \left(\int_{-\infty}^{+\infty} dx \; x \, |\psi(x)|^2\right)^2$$

Here we have assumed $\int_{-\infty}^{+\infty} dx \, |\psi(x)|^2 = 1$

$$\Rightarrow (\Delta x)^2 = \int_{-\infty}^{+\infty} dx \;\; x^2 |\psi(x)|^2 - \left(\int_{-\infty}^{+\infty} dx \;\; x \, |\psi(x)|^2 \right)^2$$

will give us the variance of the measurement of the position in the state $|\psi\rangle$.

Let us consider the following state, which we will call a Gaussian wave packet:



$$\psi(x) = A \quad e^{-(x-x_0)^2/4a^2}$$

We must normalize the state:

$$\int_{-\infty}^{+\infty} dx \;\; |\psi(x)|^2 = 1$$

$$\int_{-\infty}^{\infty} dx \;\; A^2 \quad e^{-(x-x_0)^2/2a^2} = 1$$

but $\displaystyle\int_{-\infty}^{+\infty} du \quad e^{-u^2/2a^2} = a\sqrt{2\pi}$

$\Rightarrow \quad A^2 a \sqrt{2\pi} = 1$ (note: x_0 drops out)

$$A = \left(\frac{1}{a\sqrt{2\pi}} \right)^{1/2} = \frac{1}{(2\pi a^2)^{1/4}}$$

$$\Rightarrow \quad \psi(x) = \frac{1}{(2\pi a^2)^{1/4}} \quad e^{-(x-x_0)^2/4a^2}$$

is properly normalized.

Q: What is the expectation value of $\hat{x}$ in this state ?

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{+\infty} dx \quad x \quad |\psi(x)|^2$$

$$= \int_{-\infty}^{+\infty} dx \quad x \quad A^2 \quad e^{-(x-x_0)^2/2a^2}$$

$x = x_0 + u$

$$= \int_{-\infty}^{+\infty} du \quad (x_0+u) A^2 \quad e^{-u^2/2a^2}$$

$$= x_0 A^2 a\sqrt{2\pi} + A^2 \underbrace{\int_{-\infty}^{+\infty} du \quad u \quad e^{-u^2/2a^2}}_{=0}$$

$\Rightarrow \boxed{\langle x \rangle = x_0}$ since $A^2 a\sqrt{2\pi} = 1$

Q: What is the variance of $\hat{x}$ in this state ?

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} dx \quad x^2 \; |\psi(x)|^2 = \int_{-\infty}^{+\infty} dx \; x^2 A^2 e^{-\frac{(x-x_0)^2}{2a^2}}$$

$$= \int_{-\infty}^{+\infty} du \quad (x_0+u)^2 A^2 e^{-u^2/2a^2}$$

$$= x_0^2 \Big(\underbrace{\int_{-\infty}^{+\infty} du \quad A^2 e^{-u^2/2a^2}}_{=1} \Big) + A^2 \int_{-\infty}^{+\infty} du \quad u^2 \; e^{-u^2/2a^2}$$

$$+ \; 2x_0 \underbrace{\int_{-\infty}^{+\infty} du \quad A^2 u \quad e^{-u^2/2a^2}}_{=0}$$

$$\langle x^2 \rangle = x_0^2 + \frac{1}{a\sqrt{2\pi}} \int_{-\infty}^{+\infty} du \; u^2 \, e^{-u^2/2a^2}$$

$$u = a v$$

$$\langle x^2 \rangle = x_0^2 + a^2 \int_{-\infty}^{+\infty} \frac{dv}{\sqrt{2\pi}} \; v^2 \, e^{-v^2/2}$$

$$\int_{-\infty}^{+\infty} \frac{dv}{\sqrt{2\pi}} \; e^{-\frac{v^2}{2} + i\lambda v} = e^{-\frac{\lambda^2}{2}}$$

$$\Rightarrow \int_{-\infty}^{+\infty} \frac{dv}{\sqrt{2\pi}} \; v^2 \, e^{-\frac{v^2}{2}} = \left(-i \frac{d}{d\lambda}\right)^2 \int_{-\infty}^{+\infty} dv \; e^{-\frac{v^2}{2} + i\lambda v} \Bigg|_{\lambda = 0}$$

$$= 1$$

$$\Rightarrow \langle x^2 \rangle = x_0^2 + a^2$$

$$\Rightarrow (\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$= (\cancel{x_0^2} + a^2) - (\cancel{x_0})^2$$

$$(\Delta x)^2 = a^2 \Rightarrow \boxed{\Delta x = a}$$

~~the (half {half width}~~

⇒ the half width of the Gaussian is the uncertainty in x.

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Q: What is the momentum of this state?

$$\langle p \rangle = \int_{-\infty}^{+\infty} dx \; \psi^*(x) \left(-i\hbar \frac{d}{dx}\right) \psi(x) \equiv \langle \psi | \hat{P} | \psi \rangle$$

$$= A^2 \int_{-\infty}^{+\infty} dx \; e^{-(x-x_0)^2/4a^2} \left(-i\hbar \frac{d}{dx}\right) e^{-(x-x_0)^2/4a^2}$$

$$= \frac{A^2}{2a^2} (+i\hbar) \int_{-\infty}^{+\infty} dx \; e^{-(x-x_0)^2/2a^2} (x-x_0)$$

$$= \frac{A^2}{2a^2} (+i\hbar) \int_{-\infty}^{+\infty} du \; u \; e^{-u^2/2a^2} = 0$$

$\Rightarrow \langle p \rangle = 0$ in this state.

Q: What is the variance of $\hat{p}$?

~~$(\Delta p)^2 = \int_{-\infty}^{+\infty} dx$~~ [illegible]

$$(\Delta p)^2 = \int_{-\infty}^{+\infty} dx \; \psi^*(x) \; \hat{p}^2 \; \psi(x) - \underset{0}{\langle p \rangle^2}$$

$$= -\hbar^2 \int_{-\infty}^{+\infty} dx \; \psi^*(x) \frac{d^2}{dx^2} \psi(x)$$

$$(\Delta p)^2 = \hbar^2 A^2 \int_{-\infty}^{+\infty} dx \left[+ \frac{1}{2a^2} e^{-\frac{(x-x_0)^2}{2a^2}} + \frac{1}{4a^4} (x-x_0)^2 e^{-\frac{(x-x_0)^2}{2a^2}} \right]$$

$$(\Delta p)^2 = \hbar^2 A^2 \int_{-\infty}^{+\infty} dv \left[\frac{1}{2a} e^{-v^2/2} - \frac{a^3}{4a^4} v^2 e^{-v^2/2} \right]$$

$$= \frac{\hbar^2 A^2 \sqrt{2\pi}}{4a} = \frac{\hbar^2}{4a^2}$$

$\Rightarrow \Delta p = \frac{\hbar}{2a}$ *is the variance of the measurement of the momentum*

$$\Rightarrow \Delta x \, \Delta p = \cancel{a} \frac{\hbar}{2\cancel{a}} = \frac{\hbar}{2}$$

$$\Rightarrow \boxed{\Delta x \, \Delta p = \frac{\hbar}{2}}$$

$\Rightarrow$ The state $\psi(x) = A \, e^{-(x-x_0)^2/4a^2}$ satisfies the Uncertainty Principle as an identity. These states are called *minimum spread wave packets*.

Momentum Eigenstates

Let us consider now eigenstates of the momentum operator $\hat{P}$, i.e.

$$\hat{P}\,|p\rangle = p\,|p\rangle$$

$$\Rightarrow \quad \langle x|\hat{P}|p\rangle = p\,\langle x|p\rangle$$

$$\Rightarrow \quad \psi_p(x) = \langle x|p\rangle$$

since $\langle x|\hat{P}|p\rangle = -i\hbar \frac{d}{dx}\psi_p(x)$

$$\Rightarrow \quad -i\hbar \frac{d\psi_p}{dx} = p\;\psi_p(x)$$

$$\Rightarrow \quad \psi_p(x) = A\;e^{ipx/\hbar}$$

We will choose A / $\langle p|p'\rangle = \delta(p-p')$

(orthonormality)

~~$\langle p|p\rangle = \int dx\, |\psi_p(x)|^2$~~

$$\langle p|p'\rangle = \int_{-\infty}^{+\infty} dx\;\; \psi_p(x)^*\;\psi_{p'}(x) =$$

$$= |A|^2 \int_{-\infty}^{+\infty} dx \;\; e^{-ipx/\hbar}\;\; e^{ip'x/\hbar}$$

$$= |A|^2\, 2\pi\, \delta\left(\frac{p-p'}{\hbar}\right) = |A|^2\, 2\pi\hbar\; \delta(p-p')$$

$$\Rightarrow \quad |A| = \frac{1}{\sqrt{2\pi\hbar}}$$

and

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \; e^{i\frac{px}{\hbar}}$$

These states have well defined momentum and are orthonormal.

Note: The state is defined up to an arbitrary phase $e^{i\alpha}$ which is unobservable.

Momentum Wave Packets

Let us consider states obtained by linear superposition of momentum states

$$|\psi\rangle = \int_{-\infty}^{+\infty} dp \quad \psi(p) \quad |p\rangle$$

We will assume that $\psi(p)$ is sharply peaked around a momentum p_0.

$$\Rightarrow \quad \langle x|\psi\rangle = \psi(x) = \int_{-\infty}^{+\infty} dp \quad \psi(p) \quad \langle x|p\rangle$$

$$\psi(x) = \int_{-\infty}^{+\infty} \frac{dp}{\sqrt{2\pi\hbar}} \; e^{ipx/\hbar} \quad \psi(p) \quad \left(\text{i.e. Fourier Transform}\right)$$

$$\Rightarrow \quad \langle\psi|P|\psi\rangle = \int dp \langle\psi|p\rangle p \langle p|\psi\rangle$$

$$= \int_{-\infty}^{+\infty} dp \quad |\psi(p)|^2 p$$

is the average momentum in state $|\psi\rangle$

Q: what is the average position in $|\psi\rangle$?

$$\langle\psi|\hat{X}|\psi\rangle = \int dp \int dp' \langle\psi|p\rangle\langle p|\hat{X}|p'\rangle\langle p'|\psi\rangle$$

$$= \int dp \int dp' \quad \psi(p)^* \psi(p') \quad \langle p|\hat{X}|p'\rangle$$

since $\quad [\hat{X}, \hat{P}] = i\hbar$

$$\Rightarrow \quad \langle p|[\hat{X}, \hat{P}]|p'\rangle = i\hbar \langle p|p'\rangle = i\hbar\,\delta(p-p')$$

but $\quad \langle p|\hat{X}\hat{P}|p'\rangle = \langle p|\hat{X}|p'\rangle p'$

$$\langle p|\hat{P}\hat{X}|p'\rangle = p\langle p|\hat{X}|p'\rangle$$

$$\Rightarrow \quad (p'-p) \langle p|\hat{X}|p'\rangle = i\hbar\,\delta(p-p')$$

$$\Rightarrow \quad \langle p|\hat{X}|p'\rangle = +i\hbar \frac{d}{dp}\delta(p-p') = -i\hbar \frac{d}{dp'}\delta(p-p')$$

$$\Rightarrow \langle\psi|\hat{X}|\psi\rangle = \int dp \int dp' \quad \psi(p)^* \psi(p') \quad (+i\hbar \frac{d}{dp})\,\delta(p-p')$$

$$\Rightarrow = \int dp \ \psi(p)^* (+i\hbar) \frac{d\psi(p)}{dp}$$

Finite Displacements

Consider some state $|\Psi\rangle$ whose representation in position space is $\Psi(x) = \langle x|\Psi\rangle$

Q: Can we construct a ket $|\Psi\rangle_a$ obtained by $x \to x+a$?

i.e. $\langle x|\Psi\rangle_a = \Psi(x+a)$

Let $\mathcal{U}_a$ be some (yet undetermined) linear operator s.t.

$$|\Psi_a\rangle = \mathcal{U}[a]|\Psi\rangle$$

$$\Rightarrow \quad \langle x|\Psi\rangle_a = \langle x|\mathcal{U}[a]|\Psi\rangle$$

Consider now another ket $|\Omega\rangle$ and the displaced ket $|\Omega\rangle_a$

Q. What is the relation ~~betwell~~ between

$\langle\Omega|\Psi\rangle$ and ${}_a\langle\Omega|\Psi\rangle_a$?

A. $\langle\Omega|\Psi\rangle = {}_a\langle\Omega|\Psi\rangle_a$ because space is homogeneous (i.e. no preferred origin)

$$\Rightarrow \quad \langle\Omega|\Psi\rangle = \langle\Omega|\mathcal{U}^\dagger[a]\,\mathcal{U}[a]|\Psi\rangle$$

$\Rightarrow \quad \mathcal{U}^{\dagger}[a]\,\mathcal{U}[a] = \hat{I} \quad \Rightarrow$ $\underline{\mathcal{U}[a]}$ is <u>unitary</u>

How do we find $\mathcal{U}[a]$?

Consider first an infinitesimal translation:*

$$\Rightarrow \quad \psi(x+a) = \langle x | \psi \rangle_a = \langle x | \mathcal{U}[a] | \psi \rangle$$

$$= \int dx' \langle x | \mathcal{U}[a] | x' \rangle \psi(x')$$

If a is infinitesimal $\Rightarrow$ $\psi(x+a) = \psi(x) + a\,\psi'(x) + O(a^2)$

$$\Rightarrow \quad \text{Let } \mathcal{U}[a] = \hat{I} + \cancel{a}\,\delta\hat{\mathcal{U}}\,a$$

$$\Rightarrow \quad a\,\psi'(x) = \int dx'\, a \langle x | \delta\mathcal{U}[a] | x' \rangle \psi(x')$$

$$\Rightarrow a \langle x | \delta\mathcal{U}[a] | x' \rangle = a \frac{d}{dx} \delta(x-x')$$

But $\langle x | \hat{P} | x' \rangle = -i\hbar \dfrac{d}{dx} \delta(x-x')$

$$\Rightarrow \quad \langle x | \delta\mathcal{U}[a] | x' \rangle = \frac{i\cancel{a}}{\hbar} \langle x | \hat{P} | x' \rangle$$

$\Rightarrow$ The momentum operator is the generator of infinitesimal displacements of the state.

⑨

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For finite a we use Taylor's formula

$$\psi(x+a) = \sum_{n=0}^{\infty} \frac{\psi^{(n)}(x)}{n!} a^n$$

and write

$$\mathcal{U}[a] = \sum_{n=0}^{\infty} \frac{a^n}{n!} \delta_n \mathcal{U}$$

with $\delta_0 \mathcal{U} = I$ and $\delta_1 \mathcal{U} \equiv \delta \mathcal{U}$

By inspection we see that

$$\frac{a^n}{n!} \psi^{(n)}(x) = \int dx' \frac{a^n}{n!} \langle x | \delta_n \mathcal{U} | x' \rangle \psi(x')$$

$$\Rightarrow \langle x | \delta_n \mathcal{U} | x' \rangle = \frac{d^n}{dx^n} \delta(x-x')$$

$$\Rightarrow \delta_n \mathcal{U} = \left(\frac{i}{\hbar}\right)^n \hat{P}^n$$

$$\Rightarrow \mathcal{U}[a] = \sum_{n=0}^{\infty} \frac{a^n}{n!} \left(\frac{i}{\hbar}\right)^n \hat{P}^n$$

$$\Rightarrow \boxed{\mathcal{U}[a] = e^{i\hat{P}a/\hbar}}$$

is the unitary operator we were looking for.

Suppose we want to see what is the effect of a finite translation on the expectation value of some observable. Let $\hat{A}$ be an arb. observable and $|\psi\rangle$ be some ket.

$\Rightarrow$ $\langle\psi|\hat{A}|\psi\rangle$ is the exp. value before translation and ${}_a\langle\psi|\hat{A}|\psi\rangle_a$ is the exp. value after translation. Now

$$ {}_a\langle\psi|\hat{A}|\psi\rangle_a = \langle\psi|\mathcal{U}^{-1}\hat{A}\,\mathcal{U}|\psi\rangle $$

since $|\psi_a\rangle = \mathcal{U}|\psi\rangle$ and ${}_a\langle\psi| = \langle\psi|\mathcal{U}^{+*}$
$= \langle\psi|\mathcal{U}^{-1}$

$\Rightarrow$ the translated observable is

$$ \hat{A}[a] = \mathcal{U}^{+*}\,\hat{A}\,\mathcal{U} $$

In particular if we choose $\hat{A} = \hat{X}$ (the coordinate)

$$ \Rightarrow \mathcal{U}^{+*}\hat{X}\,\mathcal{U} = e^{-i\frac{a}{\hbar}\hat{P}}\,\hat{X}\,e^{\frac{ia}{\hbar}P} = \hat{X} + a\hat{I} $$

For this reason $e^{ia P/\hbar}$ is also called a shift operator.

[$e^{-i\frac{aP}{\hbar}}\,X\,e^{ia\frac{P}{\hbar}} = X + a$ in simpler notation]

$\Rightarrow$ $\hat{P}$ generates infinitesimal translations and $e^{ia\hat{P}/\hbar}$ generates finite translation.

Note: Suppose that $\hat{A} = \hat{A}[\hat{P}]$ only

$\Rightarrow$ Since $[\hat{P},\hat{P}]=0$ and $[\hat{P}, A[\hat{P}]] = 0$

$\Rightarrow$ $\mathcal{U}^{+} A(\hat{P})\mathcal{U} = \mathcal{U}^{+}\mathcal{U} A(P) = A(P)$

$\Rightarrow$ A($\hat{P}$) is invariant under translations.

Ⓛ11

Time Evolution of Quantum States and Dynamics

We now turn to the question of the time evolution of quantum states. Let $|\psi(t_0)\rangle \equiv |\psi\rangle_{t_0}$ be some ket at time t_0 and $|\psi(t)\rangle \equiv |\psi\rangle_t$ be the ket of the system at time t. Since we want to preserve the validity of the Superposition Pple. We will assert that the evolved state is related to the initial state by the action of some linear operator $\mathcal{U}[t,t_0]$ such that

$$\Rightarrow \quad |\psi(t)\rangle = \hat{U}\{t,t_0\}\, |\psi(t_0)\rangle$$

Also we will demand that this operator $\hat{U}$ be a property of the system and hence independent of the state itself $\Rightarrow$ If $|\psi'(t_0)\rangle$ is some other state $\Rightarrow$

$$|\psi'(t)\rangle = \hat{U}(t,t_0)\, |\psi'(t_0)\rangle$$

with <u>the same</u> operator $\hat{U}$.

$$\Rightarrow \quad \langle \psi'(t) | \psi(t)\rangle = \langle \psi'(t_0) | \hat{U}^{+*}(t,t_0)\, \hat{U}(t,t_0) |\psi\rangle$$

$\psi(t_0)$

Once again we will require that

$$\langle \psi'(t) | \psi(t)\rangle = \langle \psi'(t_0) | \psi(t_0)\rangle$$

Since the origin of time should be arbitrary (time must be homogeneous) $\Rightarrow$

$$\hat{U}^{+*}(t,t_0)\, \hat{U}(t,t_0) = \hat{I} \quad \Rightarrow \hat{U} \text{ is unitary}$$

Also If $|\psi(t)\rangle = \hat{U}(t,t_0)\, |\psi(t_0)\rangle$

$$\Rightarrow \quad |\psi(t_0)\rangle = \hat{U}^{+*}(t,t_0)\, |\psi(t)\rangle$$
$$= \hat{U}(t_0,t)\, |\psi(t)\rangle$$

$$\Rightarrow \hat{U}(t,t_0) = \hat{U}^{+*}(t_0,t) = \hat{U}^{-1}(t_0,t)$$

Let us now look at infinitesimal time translations

$$|\psi(t+\delta t)\rangle = |\psi(t)\rangle + \delta t \frac{\partial}{\partial t}|\psi(t)\rangle + O((\delta t)^2)$$

Since $\hat{u}$ is unitary $\Rightarrow$ $\hat{u}^{-1} = \hat{u}^{+}$. And, since for $t' \to t$, $\hat{u}(t', t) \to \hat{I}$ $\Rightarrow$ we can write

$$\hat{u}(t+\delta t, t) = \hat{I} + i\frac{\delta t}{\hbar}\hat{H} + O((\delta t)^2)$$

where $\hat{H} = \hat{H}^{+}$ is a Hermitian operator (we have introduced $\hbar$ for further convenience)

$$\Rightarrow \ |\psi(t+\delta t)\rangle = \hat{u}(t+\delta t, t)\,|\psi(t)\rangle$$

$$|\psi(t)\rangle + \delta t \frac{\partial}{\partial t}|\psi(t)\rangle + O((\delta t)^2) =$$

$$= \left[\hat{I} + i\frac{\delta t}{\hbar}\hat{H} + O((\delta t)^2)\right]|\psi(t)\rangle$$

$$\Rightarrow \ \frac{\partial}{\partial t}|\psi(t)\rangle = \frac{i}{\hbar}\hat{H}|\psi(t)\rangle$$

or

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

Q1: what is the meaning of this equation?

i.e., what does $\hat{H}$ represent?

This equation is <u>Schrödinger's Equation of Motion for</u>

the states. If we give a definition of $\hat{H}$, this equation tells us how ~~do~~ states evolve in time. We will <u>assert</u> that $\hat{H}$ is the quantum mechanical analog of the classical Hamiltonian. The reason for this is that this quantum Hamiltonian, as an operator, generates the (infinitesimal) time evolution just as the classical Hamiltonian generates the classical time evolution. Thus we are making use of the Correspondence Pple. when we state that $\hat{H}$ is the Hamiltonian;

How do we construct this Hamiltonian? Let us try to see how much guidance we get from the correspondence pple. In classical mechanics the Hamiltonian is a function $H(q,p)$

In QM coordinates and momenta become operators which act on the Hilbert space of states $\{|\psi\rangle\}$. Hence we associate linear Hermitian operators to both q and p, which we called $\hat{Q}$ and $\hat{P}$ ($\hat{Q}$ is what we referred to as $\hat{X}$). Hence, according to the Correspondence Principle we must make the assignment

$$H(q,p) \longrightarrow H(\hat{Q},\hat{P})$$

Q: Is this assignment unique? For simple cases the Correspondence Pple. leads to a unique Quantum Hamiltonian. For example of

$$H(q,p) = T(p) + V(q)$$

$$\Rightarrow \hat{H} = T(\hat{P}) + V(\hat{Q})$$

without ambiguity.

However if for instance $T(q,p)$ is allowed (this happens in a number of cases of interest)

$\Rightarrow$ we may have different possibilities. For instance

~~if T = const~~

if T has a term of the form q^2p^2

$\Rightarrow$ we have an operator ordering ambiguity. The correspondence Pple. does not specify which ordering we should choose, aside from the requirements of Hermiticity. Thus Q^2P^2 is not Hermitian $\Rightarrow$ not allowed but QP^2Q and PQ^2P are both Hermitian and have the same correspondence limit (as does $\frac{1}{2}Q^2P^2+\frac{1}{2}P^2Q^2$). Hence it is a matter of physical definition which one is correct (or which linear combination). This rule has to be determined separately.

Similarly we will also encounter physical observables, such as spin, which have no classical analog and for which the Correspondence Ppl. has nothing to say.

Finite time Translations

The Equation of motion for the states

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H\,|\psi(t)\rangle$$

supplied with the initial condition $|\psi(t_0)\rangle$

tells us how do states evolve infinitesimally

Let us write

$$|\psi(t)\rangle = \mathcal{U}(t,t_0)\,|\psi(t_0)\rangle$$ with $|\psi(t_0)\rangle$ fixed

$$\Rightarrow i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}\mathcal{U}(t,t_0) = H\,\mathcal{U}(t,t_0)$$

Here we have assumed that H does not depend on time. In Phys. 481 we will come back to this question.

The solution to this equation is

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}$$

since $\mathcal{U}(t_0,t_0) = I$ and $\mathcal{U}^{-1} = \mathcal{U}^{+}$

where $$e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} \equiv \sum_{n=0}^{\infty} \frac{(-i)^n}{n!\,\hbar^n}(t-t_0)^n \hat{H}^n$$

Note: If $H = H(t)$ this does not quite work correctly

$$\Rightarrow \int_{t_0}^{t} dt'\, i\hbar \frac{\partial}{\partial t'}\mathcal{U}(t',t_0) = \int_{t_0}^{t} dt'\, H(t')\,\mathcal{U}(t',t_0)$$

$$\Rightarrow \; i\hbar \left(\mathcal{U}(t,t_0) - \mathcal{U}(t_0,t_0) \right) =$$

$$= \int_{t_0}^{t} dt' \; H(t')\, \mathcal{U}(t',t_0)$$

$(\mathcal{U}(t_0,t_0) = I)$

$$\Rightarrow \; \mathcal{U}(t,t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \; H(t')\, \mathcal{U}(t',t_0)$$

is an integral equation

$\Rightarrow$ if we iterate (formally)

$$\mathcal{U}(t,t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \; H(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, H(t')\, \underset{\nearrow \; \mathcal{U}(t'',t_0)}{H(t'')}$$

It is standard to define the <u>time-ordering operator</u>

$$T\, A(t)\, B(t') = \theta(t-t')\, A(t)\, B(t') + \theta(t'-t)\, B(t')\, A(t)$$

where $\theta(t-t') = \begin{cases} 1 & t > t' \\ 0 & t < t' \end{cases}$

$$\Rightarrow \mathcal{U}(t,t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' \; H(t') + \frac{1}{2!} \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt \int_{t_0}^{t} dt' \; T\, H(t')\, H(t'')$$

$$+ \cdots + \frac{1}{n!} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_n}^{t} dt_n \; T\left(H(t_1) \cdots H(t_n)\right) + \cdots$$

$$\Rightarrow \mathcal{U}(t,t_0) \equiv T \; e^{-\frac{i}{\hbar} \int_{t_0}^{t} dt' \; H(t')}$$

(which is shorthand for the long expression!)

Thus for time-independent Hamiltonians the <u>evolution operator</u> $\mathcal{U}(t,t_0)$ is

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}$$

This is the operator that maps a state at time t_0 to another state at time t.

Suppose we wish to compute the expectation value at time t of an operator (which generally depends on time) $\hat{A}(t)$ in some state $|\psi(t)\rangle$

$$\langle A(t)\rangle = \langle \psi(t)|\hat{A}(t)|\psi(t)\rangle$$

Can we find an equation of motion for this expectation value? Yes!

$$\frac{d}{dt}\langle A(t)\rangle = \left(\frac{\partial}{\partial t}\langle\psi(t)|\right)\hat{A}(t)|\psi(t)\rangle$$

$$+ \langle\psi(t)|\frac{\partial \hat{A}}{\partial t}|\psi(t)\rangle$$

~~+ [illegible]~~

$$+ \langle\psi(t)|\hat{A}(t)\left(\frac{\partial}{\partial t}|\psi(t)\rangle\right)$$

but $$\frac{\partial}{\partial t} |\psi(t)\rangle = -\frac{i}{\hbar} H |\psi(t)\rangle$$

and $$\frac{\partial}{\partial t} \langle\psi(t)| = \frac{i}{\hbar} \langle\psi(t)| H$$

$(H^{+} = H)$

$$\Rightarrow \quad \frac{d}{dt}\langle A(t)\rangle = \left\langle \frac{\partial A}{\partial t}\right\rangle + \frac{i}{\hbar}\langle HA\rangle - \frac{i}{\hbar}\langle AH\rangle$$

$$\Rightarrow \frac{d}{dt}\langle A(t)\rangle = \left\langle \frac{\partial A}{\partial t}\right\rangle + \left\langle \frac{i}{\hbar}[H, A]\right\rangle$$

or $$\frac{d}{dt}\langle A(t)\rangle = \left\langle \left(\frac{\partial A}{\partial t} + \frac{i}{\hbar}[H, A]\right)\right\rangle$$

This equation is the quantum mechanical analog of

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, H\}_{PB}$$

↳ Poisson Bracket.

We will show later on that as $\hbar \to 0$ we will get an exact correspondence. Notice that in this formulation of quantum mechanics, ~~a~~ this is an equation of motion for the expectation values of the observable. In particular let us consider the observables q and p which do not depend explicitly on t.

$$\Rightarrow \quad \frac{d}{dt}\langle q\rangle = \frac{-i}{\hbar}\langle [q, H(q,p)]\rangle$$

But $\quad q \equiv i\hbar\frac{\partial}{\partial p} \qquad$ and $\quad p = -i\hbar\frac{\partial}{\partial q}$

$$\Rightarrow \quad [q, H] = i\hbar\frac{\partial H}{\partial p}$$

(assuming there is no ordering ambiguity!)

$$\Rightarrow \quad \frac{d}{dt}\langle q\rangle = \left(\frac{-i}{\hbar}\right) i\hbar \left\langle\frac{\partial H}{\partial p}\right\rangle$$

$$\Rightarrow \quad \frac{d}{dt}\langle q\rangle = \left\langle\frac{\partial H}{\partial p}\right\rangle$$

Similarly

$$\frac{d}{dt}\langle p\rangle = \frac{-i}{\hbar}\langle [p, H(q,p)]\rangle$$

$$= \left(\frac{-i}{\hbar}\right)(-i\hbar)\left\langle\frac{\partial H}{\partial q}\right\rangle$$

$$\Rightarrow \quad \frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial H}{\partial q}\right\rangle$$

$$\Rightarrow \quad \frac{d\langle q\rangle}{dt} = \left\langle \frac{\partial H}{\partial p} \right\rangle$$

$$\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial H}{\partial q} \right\rangle$$

Eherenfest's Theorem

⇒ Hamilton's Eqns are obeyed on average

This also means that QM approaches CM if the expectation values are infinitely sharp, i.e. if $\hbar \to 0$. In particular this result also means that all the equations of Classical Mechanics are satisfied on average.

⑩ 2/21/03

L12

Schrödinger's Picture and Heisenberg's Picture

In our discussion we formulated QM in terms of a set of state vectors, kets $|\psi(t)\rangle$, which vary in time. The operators are assumed not to have any explicit time dependence. Thus the time dependence of expectation values is due entirely to the time evolution of the states themselves.

i.e.

$$\langle A(t)\rangle \equiv \langle \Psi(t)|\,\hat{A}\,|\Psi(t)\rangle$$

where

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}\,|\Psi(t)\rangle$$

This way of describing QM is called the Schrödinger picture. In this picture the expectation values of the observables obey an equation of motion, reminiscent of the classical equation of motion. We also saw that there exists ~~an~~ a linear unitary operator $\hat{\mathcal{U}}(t)$ which evolves the state $|\Psi(t_0)\rangle$ into the state $|\Psi(t)\rangle$.

There is an alternative picture due to Heisenberg (there are actually many others, but this one is special). Let us denote by $\hat{A}_S$ the operator $\hat{A}$ in the Schrödinger picture. Let $|\Psi_H(t)\rangle$ be the Heisenberg state vector, defined by

$$|\Psi_H(t)\rangle = \hat{\mathcal{U}}_S^{\dagger}(t,t_0)\,|\Psi_S(t)\rangle$$

(i.e. we go to the "moving frame")

since $|\Psi_S(t)\rangle = \hat{U}_S(t,t_0)\,|\Psi_S(t_0)\rangle$

$$\Rightarrow \quad |\Psi_H(t)\rangle = \underbrace{\hat{U}_S^{+}(t,t_0)\,\hat{U}_S(t,t_0)}_{\hat{I}}\,|\Psi_S(t_0)\rangle$$

$$\Rightarrow \quad |\Psi_H(t)\rangle = |\Psi_S(t_0)\rangle$$

$\Rightarrow$ the Heisenberg state vector is fixed in time.

$$\Rightarrow \quad \langle\Psi_S(t)|\,\hat{A}_S\,|\Psi_S(t)\rangle =$$

$$= \langle\Psi_H(t)|\,U_S^{+}(t,t_0)\,\hat{A}_S\,U_S(t,t_0)\,|\Psi_H(t)\rangle$$

$$\equiv \langle\Psi_S(t_0)|\,U_S^{+}(t,t_0)\,\hat{A}_S\,U_S(t,t_0)\,|\Psi_S(t_0)\rangle$$

$$\Rightarrow \quad \hat{A}_H(t) \equiv U_S^{+}(t,t_0)\,\hat{A}_S\,U_S(t,t_0)$$

and
$$\boxed{i\hbar\,\frac{d\hat{A}_H}{dt} = [\hat{A}_H(t),\hat{H}]}$$

$\Rightarrow$ In the Heisenberg picture the states are fixed and the operators obey equations of motion (similar to those of the Classical Theory

$$\frac{dA}{dt} = \{A, H\}.)$$

Quantum Measurements: Pure and Mixed States; Density Matrices

Let us review the concept of measurement in Quantum ~~Meta~~ Mechanics. What we mean is the following. We first imagine that the system is in a quantum state $|\psi\rangle$. Or, rather, we imagine that we will either repeat this experiment many times, always with the same state $|\psi\rangle$, or that we have an ensemble of N independent systems (copies!) all prepared in the same state $|\psi\rangle$. When we say make a certain ~~we do a~~ measurement, what we do is to project the state of the system $|\psi\rangle$ onto an eigenstate $|\omega\rangle$ of some physical observable $\hat{\Omega}$. Which observable it is, depends on our choice of measurement apparatus. In most cases we project onto a unique state. (~~But~~ in some cases, these projected states may be degenerate.) In any case the resulting state is precisely known. Such states, which are called pure states, represent according to QM, the ~~the~~ ~~~~ maximum degree of what we can know (in principle) about the physical system.

Let $\mathbb{P}_\omega = |\omega\rangle\langle\omega|$ be the projection operator onto the pure state $|\omega\rangle$. The (normalized) projected state is then

$$\frac{\mathbb{P}_\omega |\psi\rangle}{\langle \mathbb{P}_\omega \psi | \mathbb{P}_\omega \psi\rangle^{1/2}}$$

Note: projection operators obey the property $\mathbb{P}^2 = \mathbb{P}$
$\Rightarrow$ repeated measurements of the <u>same</u> observable will yield the <u>same</u> result.

What happens if we measure more than one observable? Now the result of the measurement depends on whether the $\overbrace{\text{observables, are}}^{\text{say } \Omega \text{ and } \Sigma,}$ compatible or not, i.e. whether they commute or not. If they commute and are both non-degenerate with eigenvalues ω and σ
$\Rightarrow$ the projected state is (up to normalization) $|\omega, \sigma\rangle$ and the state is unique. If however one of the observables is degenerate $\Rightarrow$ we have more than one state $|\omega_1, \sigma\rangle$ and $|\omega_2, \sigma\rangle$
If we measure $\hat{\Omega}$ first $\Rightarrow$ we $\overset{\text{(say)}}{\text{get}}$ $|\omega_1, \sigma\rangle$

Then, the result of measuring $\hat{\Sigma}$ leads to the same state since $|\omega_1,\sigma\rangle \longrightarrow |\omega_1,\sigma\rangle$ (projection)

Conversely if we first measure $\hat{\Sigma}$ we will get a linear combination $\alpha|\omega_1,\sigma\rangle + \beta|\omega_2,\sigma\rangle$ as a projected state. The normalized state is

$$\frac{\alpha\,|\omega_1,\sigma\rangle + \beta|\omega_2,\sigma\rangle}{\sqrt{\alpha^2+\beta^2}} \, , \quad \text{with probability } \alpha^2+\beta^2$$

(the square of the projection of $|\psi\rangle$)

If we now measure $\hat{\Omega}$ we get ω_1 with probability $\frac{|\alpha|^2}{\alpha^2+\beta^2}$ and ω_2 with probability $\frac{\beta^2}{\alpha^2+\beta^2}$. Thus the total probability ~~to~~ of obtaining $|\omega_1,\lambda\rangle$ is $\frac{\alpha^2}{\cancel{\alpha^2+\beta^2}}\cdot\cancel{(\alpha^2+\beta^2)} = \alpha^2$. Notice that this is the <u>same</u> probability as in the reversed order measurement.

$\Rightarrow$ we get the same answer with the same probability regardless the states are degenerate or not.

What happens if $[\hat{\Omega},\hat{\Sigma}] \neq 0$? Now we have incompatible measurements. Indeed if $[\hat{\Omega}, \hat{\Sigma}] \neq 0$ there is a generalized Uncertainty Principle at work.

Let $\hat{\Gamma} = \hat{\Gamma}^{+}$, and $\hat{\Omega}^{+} = \hat{\Omega}$, $\hat{\Sigma}^{+} = \hat{\Sigma}$ /

$$[\hat{\Omega}, \hat{\Sigma}] = i\,\hat{\Gamma}$$

Let $\langle \hat{\Omega} \rangle \equiv \langle \psi | \hat{\Omega} | \psi \rangle$ (same with $\hat{\Sigma}$ and $\hat{\Gamma}$)

for some pure state $|\psi\rangle$. Let us define the uncertainties $\Delta\Omega$ and $\Delta\Sigma$ by

$$(\Delta\Omega)^2 = \langle \psi | (\hat{\Omega} - \langle \hat{\Omega} \rangle)^2 | \psi \rangle$$

$$(\Delta\Sigma)^2 = \langle \psi | (\hat{\Sigma} - \langle \hat{\Sigma} \rangle)^2 | \psi \rangle$$

Let us denote the kets

$$|f\rangle = (\hat{\Omega} - \langle \hat{\Omega} \rangle)|\psi\rangle$$

$$|g\rangle = (\hat{\Sigma} - \langle \hat{\Sigma} \rangle)|\psi\rangle$$

$$\Rightarrow (\Delta\Omega)^2 = \langle \psi | (\hat{\Omega} - \langle \hat{\Omega} \rangle)^2 | \psi \rangle \equiv \|f\|^2$$

and

$$(\Delta\Sigma)^2 = \langle \psi | (\hat{\Sigma} - \langle \hat{\Sigma} \rangle)^2 | \psi \rangle \equiv \|g\|^2$$

where $\|f\|^2 = \langle f|f\rangle$ and $\|g\|^2 = \langle g|g\rangle$

Inner products satisfy the Schwartz Inequality:

$$\boxed{|\langle f|g\rangle|^2 \leq \|f\|^2 \|g\|^2}$$

$$\Rightarrow (\Delta\Sigma)^2(\Delta\Omega)^2 = \|f\|^2\|g\|^2 \geq |\langle f|g\rangle|^2$$

But $\langle f|g\rangle = \langle\psi|(\hat{\Omega} - \langle\hat{\Omega}\rangle)(\hat{\Sigma} - \langle\hat{\Sigma}\rangle)|\psi\rangle$

where we used that $\hat{\Omega}^+ = \Omega$ and $\langle\hat{\Omega}\rangle \in \mathbb{R}$.

$$\Rightarrow (\Delta\Omega)^2(\Delta\Sigma)^2 \geq |\langle\psi|(\hat{\Omega} - \langle\hat{\Omega}\rangle)(\hat{\Sigma} - \langle\hat{\Sigma}\rangle)|\psi\rangle|^2$$

But

$$(\hat{\Omega} - \langle\hat{\Omega}\rangle)(\hat{\Sigma} - \langle\hat{\Sigma}\rangle) =$$

$$= \frac{1}{2}\left[(\hat{\Omega} - \langle\hat{\Omega}\rangle)(\hat{\Sigma} - \langle\hat{\Sigma}\rangle) + (\hat{\Sigma} - \langle\hat{\Sigma}\rangle)(\hat{\Omega} - \langle\hat{\Omega}\rangle)\right]$$

$$+ \frac{1}{2}\left[(\hat{\Omega} - \langle\hat{\Omega}\rangle)(\hat{\Sigma} - \langle\hat{\Sigma}\rangle) - (\hat{\Sigma} - \langle\hat{\Sigma}\rangle)(\hat{\Omega} - \langle\hat{\Omega}\rangle)\right]$$

$$\equiv \hat{\Delta} + \frac{i}{2}\hat{\Gamma}$$

where $\hat{\Delta}^+ = \hat{\Delta}$ and $\hat{\Gamma}^+ = \hat{\Gamma}$

$$\Rightarrow \langle\psi|\hat{\Delta}|\psi\rangle \in \mathbb{R} \quad \text{and} \quad \langle\psi|\hat{\Gamma}|\psi\rangle \in \mathbb{R}$$

$$\Rightarrow (\Delta\Omega)^2(\Delta\Sigma)^2 \geq |\langle\psi|\hat{\Delta}|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|\hat{\Gamma}|\psi\rangle|^2$$

$$\geq \frac{1}{4}|\langle\psi|\Gamma|\psi\rangle|^2$$

⇒ we find the lower bound (it is $\geq$ only if $\langle\hat\Delta\rangle=0$)

$$(\Delta\Omega)(\Delta\Sigma)^2 \geq \frac{1}{4}\left|\langle\psi|[\hat\Omega,\hat\Sigma]|\psi\rangle\right|^2$$

or

$$\boxed{(\Delta\Omega)(\Delta\Sigma) \geq \frac{1}{2}\left|\langle\psi|[\hat\Omega,\hat\Sigma]|\psi\rangle\right| \equiv \frac{1}{2}\left|\langle\psi|\hat\Gamma|\psi\rangle\right|}$$

⇒ If $[\hat\Omega,\hat\Sigma]\neq 0 \Rightarrow \Delta\Omega\;\Delta\Sigma > 0$ uncertainty Pple.!

e.g. $\hat\Omega=\hat X$, $\hat\Sigma=\hat P$

$\Rightarrow [\hat X,\hat P]=i\hbar\,\hat I$

and $\langle\psi|[\hat X,\hat P]|\psi\rangle = i\hbar\;\langle\psi|\psi\rangle = i\hbar$

$$\Rightarrow \boxed{\Delta X\;\Delta P \geq \frac{\hbar}{2}}$$

Mixed States and Density Matrices

In theory we can always prepare a system (or an ensemble) in a pure state. In practice this is very difficult for many reasons: ① the system may not be really isolated and

~~two~~ ② in practice we may be able to prepare the system in some set of pure states, each with some probability. Let us examine first case ②.

In this case we have a set of pure states $\{|\psi_i\rangle\}$ and the system may be in each state with probability $p_i = \frac{n_i}{N}$ ($\sum_i p_i = 1$). Notice that this probability has nothing to do with QM! Such a state is called a mixed state.

Thus instead of a projection operator $|\psi\rangle\langle\psi|$ we have a matrix

$$\hat{\rho} = \sum_i p_i \, |\psi_i\rangle \langle\psi_i| \qquad \left(\text{with } p_i = \frac{n_i}{N} \right).$$

the Density Matrix. (here n_i is the # of systems in the ensemble in the pure state $|\psi_i\rangle$)

An example is the Gibbs Ensemble in Quantum Statistical Mechanics in which

$$p_i = \frac{1}{Z} e^{-E_i / k_B T}$$ where E_i is the

energy ~~and~~ in state $|\psi_i\rangle$, and T is the temperature (k_B = Boltzmann constant)

The (ensemble) average of an observable $\hat{\Omega}$ is

$$\overline{\langle \Omega \rangle} \equiv \sum_i \underset{\substack{\uparrow \\ \text{statistical} \\ \text{average}}}{p_i} \underbrace{\langle \psi_i | \hat{\Omega} | \psi_i \rangle}_{\text{QM exp. value}}$$

Notice that

$$\mathrm{tr}(\hat{\rho}\,\hat{\Omega}) = \sum_n \langle n | \hat{\rho}\,\hat{\Omega} | n \rangle$$

(where $\sum_n |n\rangle\langle n| = \hat{I}$)

$$= \sum_{n'} \sum_n \langle n | \hat{\rho} | n' \rangle \langle n' | \hat{\Omega} | n \rangle$$

If we choose $\{|n\rangle\} = \{|\psi_i\rangle\} \Rightarrow \langle n | \hat{\rho} | n' \rangle = \delta_{ii'}\, p_i$

$$\Rightarrow \mathrm{tr}(\hat{\rho}\,\hat{\Omega}) = \sum_i p_i \langle \psi_i | \hat{\Omega} | \psi_i \rangle = \langle \bar{\Omega} \rangle$$

$$\Rightarrow \langle \bar{\Omega} \rangle = \mathrm{tr}(\hat{\rho}\,\hat{\Omega})$$

For a pure state: $p_i = \delta_{ij} \Rightarrow \langle \bar{\Omega} \rangle = \langle \psi_j | \hat{\Omega} | \psi_j \rangle$
and $\hat{\rho} = |\psi_j\rangle\langle\psi_j|$

If we want the probability to get a particular value, ω, of the observable $\Rightarrow$ for a pure state $|\psi\rangle$ we have

$$P(\omega) = |\langle \omega|\psi\rangle|^2 = \langle\psi|\omega\rangle\langle\omega|\psi\rangle = \langle\psi|\hat{\mathbb{P}}_\omega|\psi\rangle$$
$$\equiv \langle\hat{\mathbb{P}}_\omega\rangle$$

$\Rightarrow$ In a mixed state

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$$\overline{P(\omega)} = tr(\hat{\rho}\,\hat{\mathbb{P}}_\omega)$$

L13 Let us now examine case ①. Let $\{|\psi_n\rangle\}$ be a complete set of states of the isolated system and $\{|\varphi_J\rangle\}$ ~~the~~ a complete set of state of the "universe". The states of the combined system (if the interaction is arbitrarily weak) have the form $|\psi_n\rangle|\varphi_J\rangle$

$$\equiv |\underset{\text{system}}{\psi_n}, \underset{\text{universe}}{\varphi_J}\rangle$$

A state can now be expanded as

$$|\psi\rangle = \sum_{n,J} c_{n,J}\, |\psi_n, \varphi_J\rangle$$

Let $\hat{Q}$ be the coordinate of the system and $\hat{X}$ the coordinates of the rest ⇒

$$\psi_i(q) = \langle q | \psi_i \rangle$$

$$\varphi_J(X) = \langle X | \varphi_J \rangle$$

$$\Rightarrow \quad \Psi(q, x) = \langle q, x | \Psi \rangle$$

$$\Rightarrow \quad \Psi(q, x) = \sum_{n,J} c_{n,J} \langle q | \psi_n \rangle \langle x | \varphi_J \rangle$$

$$= \sum_i \underbrace{\left[\sum_J c_{n,J} \, \varphi_J(x) \right]}_{= c_n(x)} \psi_n(q)$$

$$\Rightarrow \quad c_n(x) = \sum_J c_{n,J} \, \varphi_J(x)$$

Let $\hat{\Omega}$ be an observable which acts only on the states of the system ⇒

$$\hat{\Omega} = \sum_{n,n'} \Omega_{nn'} |\psi_n\rangle \langle \psi_{n'}|$$

$$= \sum_{n,n',J} \Omega_{nn'} |\psi_n, \varphi_J\rangle \langle \psi_{n'}, \varphi_J|$$

$$\langle\psi|\hat{\Omega}|\psi\rangle = \sum_{\substack{n,n'\\J,J'}} c_{n,J}^{*}\, c_{n',J'}\, \langle\varphi_J \psi_n|\hat{\Omega}|\varphi_{J'}\psi_{n'}\rangle$$

$$= \sum_{\substack{n,n'\\J,J'}} c_{nJ}^{*}\, c_{n'J'}\, \delta_{JJ'}\, \Omega_{nn'}$$

$$= \sum_{n,n'} \Big(\sum_{J} c_{nJ}^{*}\, c_{n'J} \Big)\, \Omega_{nn'}$$

Let us define the matrix $\rho_{nn'}$

$$\rho_{nn'} = \langle n|\hat{\rho}|n'\rangle = \sum_J c_{n'J}^{*}\, c_{nJ}$$

$$\Rightarrow \quad \langle\psi|\hat{\Omega}|\psi\rangle = tr(\hat{\rho}\hat{\Omega}) = tr(\hat{\Omega}\hat{\rho})$$

Note: $\hat{\rho}^{+} = \hat{\rho}$ and

$$tr\,\hat{\rho} = \sum_n \rho_{nn} = \sum_J |c_{nJ}|^2 = |\langle\psi|\psi\rangle|^2 = 1$$

$$\Rightarrow tr\,\hat{\rho} = 1$$

Since $\hat{\rho}$ is Hermitean $\Rightarrow$ its e.v.'s are real numbers

Since $tr\,\hat{\rho} = 1$ $\Rightarrow$ the sum of the e.v.'s $= 1$

$\Rightarrow$ the eigenvalues of $\hat{\rho}$ are <u>probabilities</u> ?

Let $|n\rangle$ be the n-th eigenket of $\hat\rho$ and let p_n be its eigenvalue. Consider

$$\hat\Omega = |n'\rangle\langle n'| = \sum_J |n'J\rangle\langle n'J|$$

(for some n')

$$\Rightarrow \langle\hat\Omega\rangle = \langle\psi|\hat\Omega|\psi\rangle = \sum_J |\langle\psi|n',J\rangle|^2 \geq 0$$

But

$$\langle\hat\Omega\rangle = \mathrm{tr}(\hat\Omega\hat\rho) = \sum_{m,n}\langle n|n'\rangle\langle m|\hat\rho|n\rangle\langle n'|m\rangle$$

$$= \rho_{n'n'} = P_{n'}$$

$\Rightarrow$ $P_{n'} \geq 0$

$\Rightarrow$ $\sum_n P_n = 1$ and $p_n \geq 0$

$\Rightarrow$ $\{P_n\}$ are the probabilities to have the system in state $|n\rangle$

In general we call this a mixed state. If $\hat\rho = |\psi\rangle\langle\psi|$ $\Rightarrow$ we have a pure state.

Equation of Motion for $\hat\rho$ (Schrödinger Picture)

$$\hat\rho(t) = \sum_n P_n\,|\psi_n(t)\rangle\langle\psi_n(t)|$$

where

$$i\hbar \frac{\partial}{\partial t} | \psi_n(t)\rangle = \hat{H} \; |\psi_n(t)\rangle$$

Since $$-i\hbar \frac{\partial}{\partial t} \langle \psi_n(t)| = \langle \psi_n(t)| \; \hat{H}$$

$$\Rightarrow \quad \frac{\partial \hat{\rho}}{\partial t} = \Sigma_n \, p_n \; \frac{\partial}{\partial t} |\psi_n(t)\rangle \; \langle \psi_n(t)|$$

$$+ \; \Sigma_n \; p_n \quad |\psi_n(t)\rangle \frac{\partial}{\partial t} \langle \psi_n(t)|$$

$$= \Sigma_n \; p_n \left[\frac{1}{i\hbar} \quad \hat{H} \; |\psi_n(t)\rangle \; \langle \psi_n(t)| \right.$$

$$\left. - \frac{1}{i\hbar} \; |\psi_n(t)\rangle \quad \langle \psi_n(t)| \, \hat{H} \right]$$

$$\Rightarrow \quad \frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} \left(\hat{H} \hat{\rho} - \hat{\rho} \hat{H} \right)$$

$$\boxed{i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\, \hat{H}, \hat{\rho}\,]}$$

Equation of motion of $\hat{\rho}$
(note: this is still the Schrödinger picture!)

and

$$\frac{d}{dt} \langle \hat{\Omega} \rangle = \left\langle \frac{\partial \hat{\Omega}}{\partial t} \right\rangle + \frac{1}{i\hbar} \; \mathrm{tr}\left([\hat{\Omega}, \hat{H}] \hat{\rho} \right)$$

Two level systems: a simple quantum mechanical system

We will now discuss the basic ideas of QM in the context of the simplest quantum mechanical system, a two-level system. For the sake of concreteness we will have in mind a system such as a single photon of momentum $\vec{p}$ and energy $E = \hbar\omega = h\nu = c\frac{h}{\lambda} = |\vec{p}|c$. Photons come in two polarization states. Let the vector $\begin{pmatrix}1\\0\end{pmatrix}$ represent a photon polarized along the x axis and $\begin{pmatrix}0\\1\end{pmatrix}$ a photon polarized along the y axis ($z \parallel \vec{p}$ is the axis of propagation). Hence a generic polarization state is

$$|\Psi\rangle = \Psi_x\, |x\rangle + \Psi_y\, |y\rangle$$

where $|x\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|y\rangle = \begin{pmatrix}0\\1\end{pmatrix}$

We will normalize these states to $\langle\Psi|\Psi\rangle = 1$

$$\Rightarrow \ |\Psi_x|^2 + |\Psi_y|^2 = 1 \qquad \text{since} \quad \langle 2|1\rangle = 0$$

and $\langle 1|1\rangle = \langle 2|2\rangle = 1$

The classical energy of an electromagnetic wave is

$$\mathcal{E} = \int_V d^3x \; \frac{1}{2} \left(\vec{E}^2(\vec{x},t) + \vec{B}^2(\vec{x},t) \right)$$

If the wave propagates along the z axis $\Rightarrow$

$$\vec{B} = \hat{z} \times \vec{E} \quad \Rightarrow \quad \vec{E}^2 + \vec{B}^2 = 2\vec{E}^2$$

such waves have the form

$$E_x(\vec{x},t) = |E_x| \cos(kz - \omega t + \varphi_x)$$

$$E_y(\vec{x},t) = |E_y| \cos(kz - \omega t + \varphi_y)$$

If the volume is very large ($V \gg \lambda^3$) $\Rightarrow$

$$\int d^3x \; \vec{E}^2 = \frac{1}{2} (E_x^2 + E_y^2) \, V$$

$$\Rightarrow \mathcal{E} = \frac{V}{2} (|E_x|^2 + |E_y|^2)$$

Let $E_x = |E_x| \, e^{i\varphi_x}$ $\qquad E_y = |E_y| \, e^{i\varphi_y}$

$\Rightarrow \vec{E} = (E_x, E_y)$ (complex components)

and

$$\mathcal{E} = \frac{V}{2} |\vec{E}|^2$$

For the case of a "single photon" wave, we must have $\mathcal{E} = \hbar\omega$

$$\Rightarrow \frac{V}{2}|\vec{E}|^2 = \hbar\omega$$

$$|\vec{E}|^2 = \frac{2}{V}\hbar\omega$$

Let $\psi_x = \dfrac{E_x}{|\vec{E}|} = E_x\sqrt{\dfrac{V}{2\hbar\omega}}$

and $\psi_y = \dfrac{E_y}{|\vec{E}|} = E_y\sqrt{\dfrac{V}{2\hbar\omega}}$

$\Rightarrow$ ψ_x represents the x-component of $\vec{E}$ and ψ_y the y-component of $\vec{E}$.

Since $\langle\psi|\psi\rangle = 1 \rightarrow |\psi_x|^2 + |\psi_y|^2 = 1$

$$\Rightarrow \psi_x = \frac{1}{\sqrt{2}}e^{i\varphi_x} \quad \text{and} \quad \psi_y = \frac{1}{\sqrt{2}}e^{i\varphi_y}$$

Notice that only $\varphi_x - \varphi_y$ has real meaning for us.

Examples:

$|x\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ x-polarized photon

$|y\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ y-polarized photon

$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$ RCP photon

$|L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$ LCP photon.

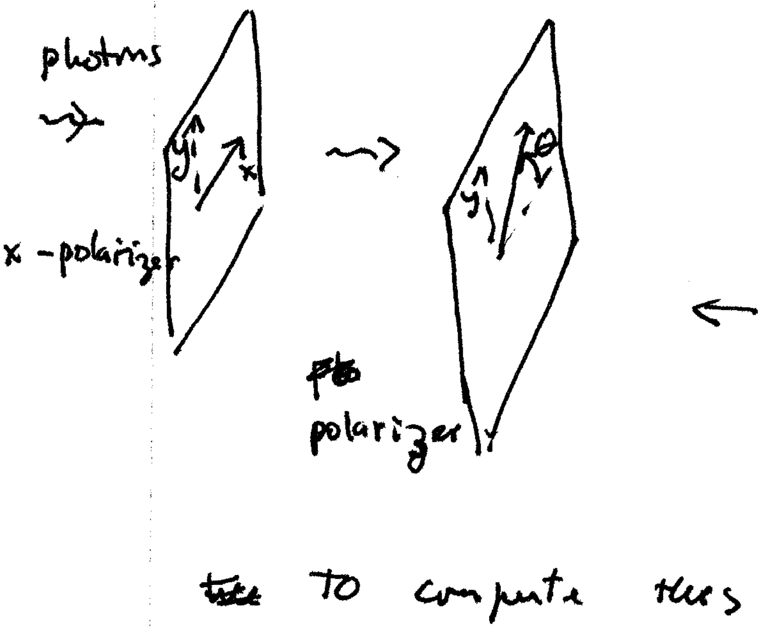
Note: the states $|x\rangle, |y\rangle$ form an orthonormal basis. The states $|R\rangle, |L\rangle$ also form an orthonormal basis.

Suppose we prepare a photon in the state

$$|\psi\rangle = \psi_x|x\rangle + \psi_y\, |y\rangle$$

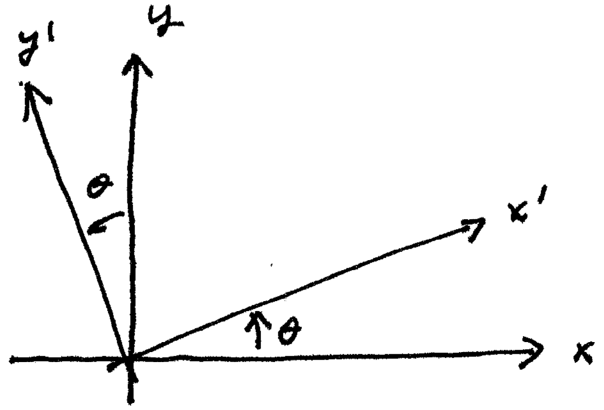
Q: what is the probability to detect an x-polarized photon? A: $|\langle x|\psi\rangle|^2 = |\psi_x|^2$ is the probability.

In particular if $|\psi\rangle = |R\rangle$ the probability to detect the photon as being x-polarized is $|\langle x|R\rangle|^2 = \frac{1}{2}$



Suppose we now take x-polarized photons, whose state is $|x\rangle$, and ask for the probability ~~that~~ to be polarized along an axis on an angle θ

~~take~~ TO compute this probability we will now rotate the state by the angle θ.



The state $|\psi\rangle$ in the new basis is

$$|\psi\rangle = \psi_{x'} |x'\rangle + \psi_{y'} |y'\rangle$$

Q: How do we relate $(\psi_{x'}, \psi_{y'})$ to (ψ_x, ψ_y)?

A: By an unitary transformation!

$$\psi_{x'} = \langle x'|\psi\rangle = \langle x'|x\rangle\langle x|\psi\rangle + \langle x'|y\rangle\langle y|\psi\rangle$$

where we used $\hat{I} = |x\rangle\langle x| + |y\rangle\langle y|$

$$\Rightarrow \psi_{x'} = \langle x'|x\rangle\, \psi_x + \langle x'|y\rangle\, \psi_y$$

$$\Rightarrow \psi_{y'} = \langle y'|x\rangle\, \psi_x + \langle y'|y\rangle\, \psi_y$$

$$\begin{pmatrix} \psi_{x'} \\ \psi_{y'} \end{pmatrix} = \begin{pmatrix} \langle x'|x\rangle & \langle x'|y\rangle \\ \langle y'|x\rangle & \langle y'|y\rangle \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix}$$

$$\Rightarrow |x\rangle = \cos\theta\, |x'\rangle - \sin\theta\, |y'\rangle$$

$$|y\rangle = \sin\theta\, |x'\rangle + \cos\theta\, |y'\rangle$$

$$\Rightarrow \langle x'|x\rangle = \cos\theta \quad , \quad \langle y'|x\rangle = -\sin\theta$$

$$\langle x'|y\rangle = \sin\theta \quad , \quad \langle y'|y\rangle = \cos\theta$$

$$\begin{pmatrix} \psi_{x'} \\ \psi_{y'} \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} \equiv R(\theta) \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix}$$

$\Rightarrow$ $R(\theta)$ is a rotation matrix and

$$R^{-1}(\theta) = \cancel{R(\theta)}\ R(-\theta) = R^{+}(\theta)$$

Q: What are the eigenvectors and eigenvalues of $R(\theta)$?

A: $$R(\theta)\,|\psi\rangle = c\,|\psi\rangle$$

We write

$$R(\theta) = \cos\theta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\sin\theta \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and verify that

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} |R\rangle = |R\rangle \qquad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} |R\rangle = |R\rangle$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} |L\rangle = |L\rangle \qquad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} |L\rangle = -|L\rangle$$

$$R(\theta)\,|R\rangle = e^{i\theta}\,|R\rangle$$

$$R(\theta)\,|L\rangle = e^{-i\theta}\,|L\rangle$$

$\Rightarrow$ Under a change of basis $|R\rangle$ and $|L\rangle$ change only by a phase factor $e^{\pm i\theta}$ (θ: angle of rotation)

Our question was to find the probability to detect the photon, originally in state $|x\rangle$, along the state $|x'\rangle \Rightarrow |\langle x'|x\rangle|^2 = \cos^2\theta$ is the probability we were looking for.

L14 Angular Momentum

We just saw that the states $|R\rangle$ and $|L\rangle$ have the interesting property that $R(\theta)|R\rangle = e^{i\theta}|R\rangle$
$R(\theta)|L\rangle = e^{-i\theta}|L\rangle$

Since $\hat{R}(\theta)$ is unitary $\Rightarrow \exists\ \hat{S} \ni /\ \hat{S}^\dagger = \hat{S}$

and $\hat{R}(\theta) = e^{i\theta\hat{S}}$

What is $\hat{S}$?

We know that $\hat{R}(\theta) = \cos\theta\ \hat{I} + i\sin\theta \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Check $\hat{S} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\hat{S}^\dagger = \hat{S}$ and $\hat{S}^2 = \hat{I}$

$$e^{i\theta\hat{S}} = \sum_{n=0}^{\infty} \frac{i^n\theta^n}{n!}\hat{S}^n = \sum_{r=0}^{\infty} \frac{i^{2r}\theta^{2r}}{(2r)!}\hat{I}$$

$$+ \sum_{r=0}^{\infty} \frac{i^{2r+1}\theta^{2r+1}}{(2r+1)!}\hat{S} = \cos\theta\ \hat{I} + i\sin\theta\ \hat{S} \quad \checkmark$$

$\Rightarrow$ The eigenstates of $\vec{S}$ are circularly polarized photons and the eigenvalues of $\vec{S}$ are ± 1.

We will now see that this property is related ~~the~~ to the angular momentum, or helicity, of the wave (and hence, the photon).

Classically the angular momentum carried by the e.m. wave is

$$\vec{L} = \frac{1}{c} \int d^3x \ \vec{r} \times (\vec{E} \times \vec{B})$$

Since $\vec{\nabla} \cdot \vec{E} = 0$ (no free charges)

$\Rightarrow$ in the Coulomb gauge $(A_0 = 0 \text{ and } \vec{\nabla} \cdot \vec{A} = 0)$

we wrote

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad \text{and} \quad \vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}$$

$\Rightarrow$ for an infinite wave we get

$$L_z = \frac{1}{c} \int d^3x \ (E_x A_y - E_y A_x)$$

(up to surface terms)

$$\Rightarrow \quad L_z = \frac{V}{2i\omega} \left(E_x^* E_y - E_x E_y^* \right)$$

$$\Rightarrow \quad L_z = \frac{V}{2\omega}\left(\left|\frac{E_x - iE_y}{\sqrt{2}}\right|^2 - \left|\frac{E_x + iE_y}{\sqrt{2}}\right|^2\right)$$

If the beam is a superposition of RCP and LCP waves $\Rightarrow$

$$\frac{E_x - iE_y}{\sqrt{2}} = E_{RCP}$$

$$\frac{E_x + iE_y}{\sqrt{2}} = E_{LCP}$$

$$L_z = \frac{V}{2\omega}\left(|E_{RCP}|^2 - |E_{LCP}|^2\right)$$

Since $E_x = \sqrt{\frac{2\hbar\omega}{V}}\,\psi_x$ and $E_y = \sqrt{\frac{2\hbar\omega}{V}}\,\psi_y$

$$\Rightarrow \quad E_{RCP} = \sqrt{\frac{2\hbar\omega}{V}}\,\psi_R \qquad E_{LCP} = \sqrt{\frac{2\hbar\omega}{V}}\,\psi_L$$

$$L_z = \frac{\cancel{V}}{\cancel{2\omega}}\,\frac{\cancel{2}\hbar\cancel{\omega}}{\cancel{V}}\left(|\psi_R|^2 - |\psi_L|^2\right)$$

$$\Rightarrow L_z = \hbar\left(|\psi_R|^2 - |\psi_L|^2\right) = \langle\psi|\,\hat{L}_z\,|\psi\rangle$$

$\Rightarrow \boxed{\hat{L}_z = \hbar\,\hat{S}}$ is the quantum mechanical operator which measures the photon helicity (or spin) along the direction of propagation $\hat{z}$.

We will return to this in Phys. 481

$\Rightarrow$ RCP photons carry angular momentum $\hbar$ and LCP photons carry angular momentum $-\hbar$

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Upolarized Light

We have considered so far photons in pure states. Suppose we prepare our single photon beam in a mixed state with p_1 the probability that the system is in state $|\psi_1\rangle$ and p_2 the probab. for state $|\psi_2\rangle$. We must now construct a density matrix. In the basis $|\psi_1\rangle$, $|\psi_2\rangle$ (which we assume is orthonormal) the density matrix is

$$\hat{\rho} = p_1 \, |\psi_1\rangle\langle\psi_1| + p_2 |\psi_2\rangle\langle\psi_2|$$

What is the probability P_x to find the photon to be x-polarized?

$$P_x = \operatorname{tr}\left(\hat{\rho} \, |x\rangle\langle x|\right)$$

$$= p_1 \, |\langle x|\psi_1\rangle|^2 + p_2 \, |\langle x|\psi_2\rangle|^2$$

Suppose for instance that $|\psi_1\rangle = |R\rangle$ and $|\psi_2\rangle = |L\rangle$

$$\Rightarrow P_x = p_1 \, |\langle x|R\rangle|^2 + p_2 \, |\langle x|L\rangle|^2 = \frac{p_1 + p_2}{2} = \frac{1}{2}$$