Preface to Write-ups

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I post with this preface two write-ups on quantum mechanics (QM) basically addressed to under-graduste, post graduate students and teachers. People involved in research may also want to refer to these write-ups. A large part of the first write-up may be appreciated by amature scientists and engineers with diverse scientific interests.

Basic idea in these notes is to address the "sticky areas" where students are stuck and grapple as they go through a course and/or a text book and finally may live with gaps in their understanding. These write-ups are not written with a view to compile them to produce a book, but each of them addresses a specific issue, complementing the development of the subject in a course or a text book.

In the first write-up I have obtained the basic concepts from the analysis of the associated experiments and also developed some skeleton theoretical structure as a consequence of the basic principles. In the second write-up, I develop all the essential aspects of mixed states and density operators, (except reduced density operators which require states of multipartite quantum systems), which is an extremely important part of QM, but surprisingly neglected in most of the courses on QM, at least in India.

For the readers : Please feel free to send me your questions/suggestions/comments. Please point out mistake(s), if you find any.

Document I
QUANTUM STATES[*]

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Contents

1 States of motion of a classical system

What do we understand by the state of a physical system at a given time? We can safely say that such a state has to be related somehow to the values of various measurable physical quantities (position, momentum, energy, angular momentum, magnetic moment etc) that turn up if we measure these quantities on the system at that time. Since these values of various physical quantities can change with time due to the interaction of the system with other systems, its state also changes with time. In a non-relativistic theory these interactions are incorporated as forces on the system. The resulting change of state in time is then connected to these forces (or the corresponding potentials if the forces are conservative) via the equations of motion. Once we know the state of the system at a given time, by making appropriate measurements at that time, we have to solve the equation of motion with these values as the initial conditions. The solution of this initial value problem tells us how does this state evolve in time as long as the pattern of forces remains the same.[1] This is the basic programme of non-relativistic physics.

Every act of measurement involves interaction between the apparatus and the system. This invariably leads to random fluctuations in the measured values. Thus if we prepare N identical systems in the same state and measure the same physical quantity, say x, then the N values $x_i,\ i = 1, \dots, N$ that turn up in these N measurements are not found to be identical. If the system is massive as compared to a single atom or a molecule and if N is large, then the observed values are found to be distributed as a bell shaped curve, (normal distribution), symmetrically around the mean

$$\langle x \rangle = \sum_{i=1}^{N} x_i/N, \tag{1}$$

whose width at half maximum or its standard deviation is

$$\Delta x = +\sqrt{\langle x^2 \rangle - \langle x \rangle^2}. \tag{2}$$

Thus the observed value of this quantity x in the given state is $\langle x \rangle$ which is uncertain by an amount $\pm\Delta x$, that is, a value of x which differs from the average value $\langle x \rangle$ by an amount less than $|\Delta x|$ cannot be taken to be a value of x different from $\langle x \rangle$ and does not define any new state apart from that defined by $\langle x \rangle$.

To understand why the observed values of a physical quantity x are distributed normally (Gaussian distribution), we note that the measuring probe comprises enormous number of atoms/molecules ($10^{21}/\mathrm{cm}^3$) that randomly jostle around their equilibrium positions. These random vibrations are independent of each other and have identical

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[1] Thus we see that in order to know the state of the system at a given time via the equation of motion, we must know its state at some previous instant of time which can only be found by measuring the state at that time. This makes the process of measurement fundamental to all of physics.

probability distributions. Since these vibrating atoms are typically on a lattice, coupled tightly together (apart from small random vibrations around their lattice positions) their response to the system in an act of measurement has a large common part, superposed on which are the small fluctuations due to their random vibrations. The net random deviation in the measured reading (typically displacement of a pointer) is then due to addition of tiny individual random fluctuations of these atoms. The observed value can be treated as the value of a random variable which is the sum of enormous number of identically distributed and independent random variables. The essential property of such a random variable which is the resultant of a large number of additive, identically distributed and independent random variables is that its probability density function [2] assumes the Gaussian form. This result is famously known as the central limit theorem. In Appendix A we give an example of the sum of identically distributed random variables tending to a Gaussian.

Let us consider an object whose rest mass is far greater than that of a single atom or a molecule. Such an object is known to fall within the purview of classical physics. An object with rest mass of 1 mg easily satisfies this condition since its mass is of the order of the mass of 10^{21} hydrogen atoms. Further, let us assume that this object is in thermodynamic equilibrium with its environment. From our experience of measuring different physical quantities on such a system, we can make following two assumptions.

- For a large number of repetitions, N, of the measurement of a quantity x, under identical conditions, the N measured values are distributed in a normal (Gaussian) distribution peaked at the average value $\langle x\rangle$ as defined above. For large N, the standard deviation Δx is negligibly small (see appendix A).
- Under identical conditions, the same value of the quantity x, (given by the average $\langle x\rangle$ of N observations), turns up, with acceptable uncertainty, irrespective of the method of measurement.

From these observations, people accept the following statements as one of the basic tenets of classical physics.[3]

At every instant of time, a classical system possesses definite values of kinamatical quantities such as its position and momentum, in the same sense as it possesses the values

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[2] The probability density function is defined as follows. Let x be a continuous random variable taking real values. Let a function $f(x)$ satisfy $f(x) \geq 0 \; \forall x$ and $\int_a^b f(x)dx$ exists for every interval $[a, b]$ within its domain. Then $f(x)$ is the density function for x if for every interval $[a, b]$ the probability that $x \in [a, b]$ is

$$P(a \leq x \leq b) = \int_a^b f(x)dx.$$

In particular, the probability that $x \in [x_0, x_0 + dx]$ is $f(x_0)dx$.

[3] This para in italics must be read carefully.

of its intrinsic properties like its mass and charge, independent of whether we attempt to measure them. The basic difference between the kinamatical quantities and the intrinsic properties is that the values of the kinamatical quantities can and in general, will change with time.[4] *Just as we say 'the charge on this particle is such and such', we can also say 'the momentum of this particle at some given time was such and such'. The values of all measurable physical quantities possessed by the system at a given time will simply be revealed by the act of measurement at that time. In principle, it is always possible to devise a measurement of a physical quantity* x *such that the corresponding uncertainty* Δx *does not affect any analysis and conclusions based on the measured (average) value* $\langle x \rangle$ *of* x*. In other words, the uncertainty* Δx *in* x *can be reduced below any required value, there is no lower bound, at least in principle. Thus any act of measurement just reveals the values of the quantities being measured, as possessed by the system at that time, without influencing these values in any way.*

This fundamental tenet of classical physics tells us that the state of a classical system at a given time can be specified by simply listing out the values of all the relevant physical quantities possessed by the system at that time. With this definition of the state of a classical system, the fundamental tenet just says that a classical system is in a unique and definite state at every instant of time, independent of whether we measure it or not.

It turns out that the state of a classical particle is completely specified by giving the values of only two vector quantities, its position $\mathbf{x}$ and momentum $\mathbf{p}$. This is because the values of all other dynamical physical quantities like angular momentum ($\mathbf{x} \times \mathbf{p}$) and energy ($\mathbf{p}^2/2m + V(\mathbf{x})$) are given functions of the values of position and momentum. If a system consists of many particles, then its state gets completely specified by giving the position and momentum of every particle in it. Since the position and momentum can be measured with any required accuracy, each particle has a definite trajectory, with a definite momentum vector at every point on the trajectory, tangent to the trajectory at that point. Equivalently, the state of a N-particle system at a given time can be specified by a point in its phase space, which is a $6N$ dimensional space with each of its points having $6N$ coordinates, $3N$ specifying the positions of the particles, while the other $3N$ coordinates specify their momentum components. A trajectory in its phase spase completely describes the temporal evolution of the system. For systems with very large number of particles, positions and momenta of individual particles are inaccessible and states of the system have to be specified by macroscopic parameters like volume, pressure, internal energy etc. Another example of a classical system which defies the program of finding the evolution of its state via its equation of motion coupled to its experimentally determined initial state is chaotic system, whose phase space trajectories emerging from arbitrarily close points corresponding to arbitrarily small error in determining its initial state diverge exponentially.

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[4] The values of the kinamatical quantities like position and momentum are relative to the inertial reference frame with respect to which they are measured. However, it is enough to know these values with respect to only one such frame : the corresponding values with respect to other inertial frames can be obtained using their relative velocities [1].

In some situations, we may not have enough information to specify the exact state of the system at a given time. Examples are chaotic systems, weather, fluids in general. The best we can say is that the system is in the state S_1 with probability $p_1, \dots,$ in the state S_k with probability $p_k, \dots,$ in the state S_N with probability p_N. However, it is very important to remember that *the system is actually in exactly one of the N states $S_1, \dots, S_N$ at a given time, and not simultaneously in more than one of these states.* The set of N states $S_1, \dots, S_N$ with corresponding probabilities have to be invoked because of our ignorance about exactly which of these states the system is in. In such a situation it is convenient to specify the state by the ensemble $\{S_k, p_k\}$, which stands for M mental copies [5]of the system with m_1 in state $S_1, \dots,$ m_k in state $S_k, \dots,$ m_N in state S_N, such that $(m_k/M) = p_k,\ k = 1, \dots, N$. The last equations are taken to be exact in the limit $M \to \infty$. The state of any system specified by the ensemble $\{S_k, p_k\}$ as defined in this paragraph is called 'classical mixture' or 'proper mixture'. In fact we will deal with the classical mixture of quantum states, bred out of our ignorance about exactly which out of a set of the quantum states the quantum system is in.

2 Quantum systems

What can we say about the states of a quantum system? We expect that a state of a quantum system must be characterized somehow by the values of the measurable physical quantities which turn up when measured on the system. For a classical system, the state is characterized simply by listing out the values of all measurable physical quantities possessed by the system in that state. But this is possible if the system has definite values of all measurable physical quantities at every instant of time. Does a quantum system satisfy this condition? Is it true that all measurable physical quantities can be regarded as some intrinsic properties of a quantum system whose values possessed by the system at a given time are simply revealed in an act of measurement and the disturbance due to measurement can be made as small as required? The answer to this question has to be obtained by designing and carrying out suitable experiments on a quantum system. We are addressing here a fundamental question regarding the behavior of quantum systems whose answer cannot be derived from some more fundamental axioms about quantum systems.

For simplicity, let us consider a single quantum particle. The state of a classical particle at a given time is specified by the definite values of particle's position and momentum vectors at that time. Can we simultaneously specify the values of both, the position and the momentum of the quantum particle? What experiment can we design to answer such a question? It turns out that we can design an experiment in response to an equivalent question. If the position $\mathbf{x}(t)$ and the momentum $\mathbf{p}(t) = m\dot{\mathbf{x}}(t)$ are both precisely known at a time t then particle's position at $(t+\Delta t)$ is known to any given accuracy via $\mathbf{x}(t+\Delta t) =$

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[5] We have to deal with mental copies, rather than actually identically prepared systems to avoid their mutual interactions which can change the states of the systems.

$\mathbf{x}(t) + \Delta t \dot{\mathbf{x}}(t)$ by suitably choosing Δt. Thus we can construct the path of the particle as a differentiable curve $\mathbf{x}(t)$ as a vector valued function of t, $(t \to \mathbf{x}(t))$ with the tangent velocity vector $\dot{\mathbf{x}}(t)$ at each point $\mathbf{x}(t)$ on the path. Conversely, if the particle is moving on a path which is a differentiable curve $\mathbf{x}(t)$, then its velocity vector $\dot{\mathbf{x}}(t)$ can be obtained at every position $\mathbf{x}(t)$ of the particle by evaluating $\dot{\mathbf{x}}(t)$ at that point. Thus a particle moves on a definite differentiable curve $\mathbf{x}(t)$ if and only if its position and momentum are simultaneously known for all time t as long as it is moving along its path. Thus the equivalent question we have to answer is : Does a quantum particle have a definite differentiable path? The corresponding experiment, famously known as the double slit experiment, not only answers this question but makes inroads for the understanding of a state of a quantum particle.

3 Double slit experiment : wave particle duality

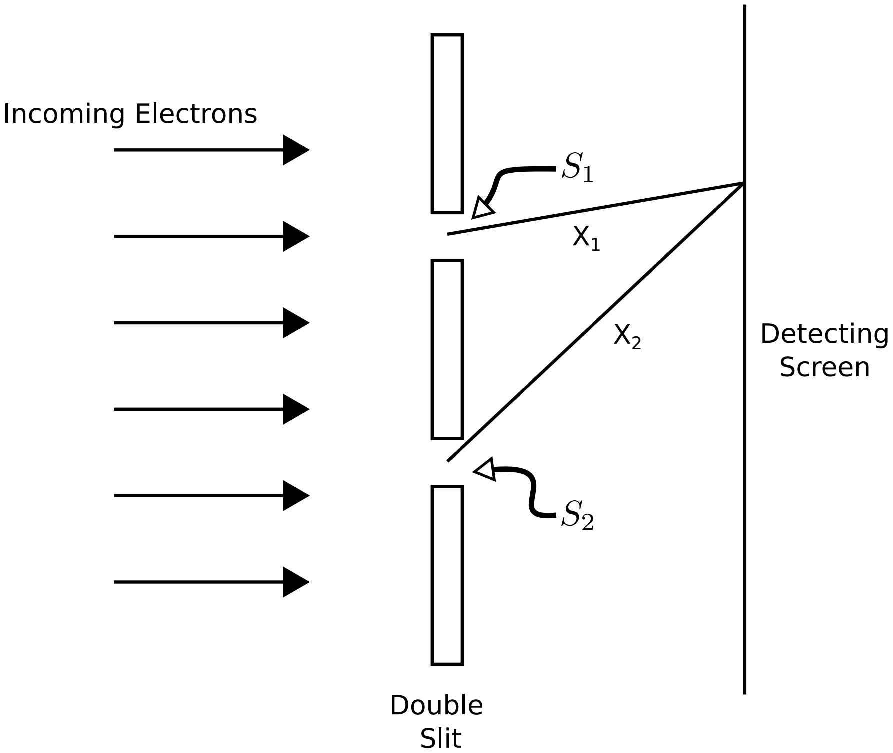

Figure 1: Schematic arrangement of the double slit experiment.

The double slit experiment was originally conceived as a thought experiment, but has been realized in a laboratory by now [2]. Thus we can describe the actual experiment and its results and discuss implications of these results.

Fig.1 shows the schematic arrangement of this experiment. Electrons strike a diaphragm with two slits so that electrons can pass through these two slits. Electrons passing through the slits hit the detecting screen and the points at which they hit the screen are recorded. The experimental conditions are arranged in such a way that there is at most one electron within the apparatus at any instant of time. This can simply be done by adjusting the emission rate of the electrons by its source. If the source produces 1000 electrons/sec at 50 KV, their average speed is about 10^8m/s. Neglecting the probability that the source emits two or more electrons simultaneously, two successive electrons are emitted at an average interval of 10^{-3} seconds. Therefore, moving at the speed of 10^8m/s, two successively emitted electrons are separated by 100km! This ensures that there is at most one electron in the apparatus at any given time. By the time the next electron arrives, the previous electron has already struck the detecting screen and its data are recorded.

3.1 Observations and their analysis

After passing through the slits, an electron strikes the detecting screen at one point, which means that electron strikes the screen as a localized lump or a particle, as expected. However, when we display the cumulative record of a large number of such strikes, (say 100 thousand) we clearly see a pattern of alternating bright and dark bands. Such patterns are known to be due to the interference of two waves, emanating from two sources. Two sources could be easily possible if many electrons were present within the apparatus at the same time. But the experiment is carried out such that no two or more electrons can be present in the apparatus at the same time. Thus a single electron is required to produce two interfering signals from the two slits. Since the electron is the one that is detected on the screen, the above requirement means that a single electron has to pass through both the slits simultaneously.

We can give an experimental evidence of the same conclusion in the following way. We carry out the experiment with say slit S_1 closed and only slit S_2 open (see Fig.2). After building up the statistics we see that the bright-dark band interference pattern is now replaced by a single broad band, with its peak across slit S_2. This implies that, in the original experiment, (when both slits were open), the electrons must be passing through slit S_1. If electrons were not passing through this slit, closing it would have made no difference. If we now block slit S_2, keep slit S_1 open and carry out the experiment, the accumulated data shows a single broad band peaking across slit S_1. This shows that the electrons must be passing through slit S_2 in the original experiment. Since there was only one electron passing through the slits at a time and passage of successive electrons through the slits are independent events, we conclude that each electron was passing through both the slits in the experimental apparatus.

This behavior is very weird. An electron is a particle, which means that it is something which is at a particular point in space. If electron is a particle, then it can be at one of the two places but never at both the places at once. But the electron in this experiment

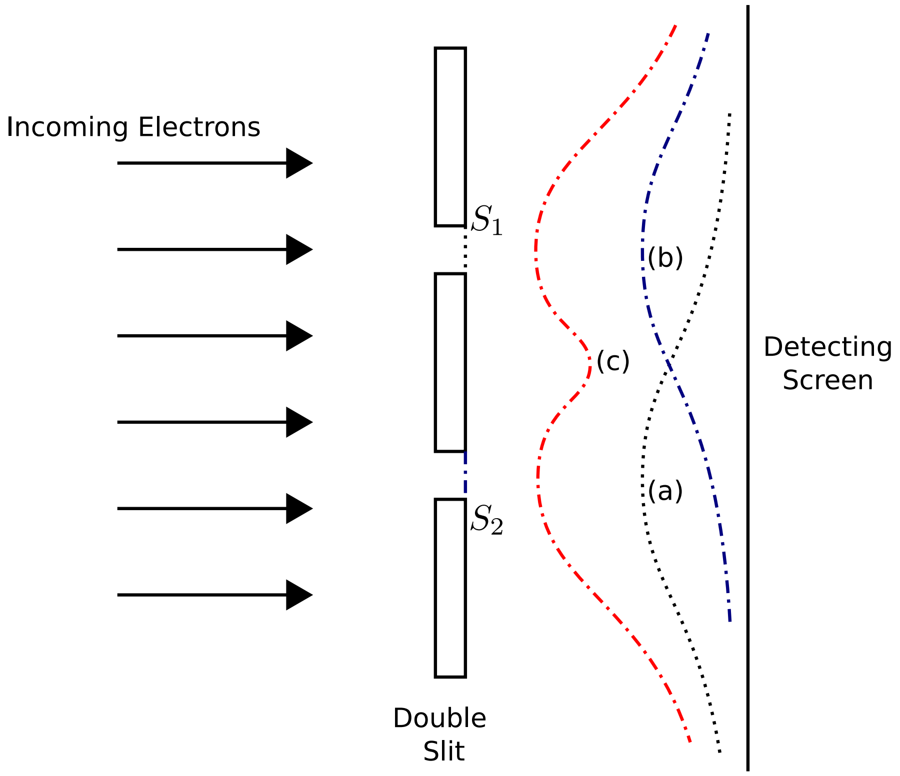

Figure 2: The observed distribution of particles (a) when S_1 is closed and S_2 is open, (b) when S_2 is closed and S_1 is open and (c) The classically expected distribution when both the slits are open.

seems to be doing just that.

3.1.1 Locality

Is there any other interpretation of the observed interference pattern in which the electron is not required to pass through both the slits at once? Yes, there is, but then we have to compromise with another fundamental axiom basic to all physics, namely locality. We concluded about the passage of an electron through both the slits at once when we noticed that closing one of the slits changes the pattern of arrivals of the electrons at the detecting screen. If the electrons were not passing through this slit, closing it would not be of any effect. This logic stands as long as we assume locality, that is, closing of one slit has no effect on electrons passing through the other one. Suppose an electron has a smooth and definite trajectory that goes through either slit S_1 or slit S_2 but not both. However, the electron trajectory through a slit depends on whether the other slit is open or closed. Then this dependence may be changing the electron trajectory giving the interference pattern when both slits are open, to the other kind of trajectories which produce the observed single band when one of the slits is closed. This is a non-local behavior : action at one place changes the course of development at the other. Thus if we accept such a non-local behavior *as an axiom,* we can produce a theory which can consistently explain all the observed quantum phenomena including the double slit experiment. Such a theory was first proposed and developed by David Bohm, and is called Bohemian Mechanics. We have no intension to study it. However, we wish to make the following comment.

As we will see in a later write-up, two or more quantum particles can be in a state which cannot be decomposed in terms of the states of individual particles. Such a state is called an entangled state, in which the particles can exhibit non-local behavior. This non-locality is a consequence of the state being entangled, which in turn is a consequence of the fundamental structure of quantum mechanics. However, in Bohmian mechanics, non-locality is included in the fundamental axioms of the theory. Non-locality pervades all Bohmian mechanics, but not all quantum mechanics. In Bohmian mechanics even the dynamics of a single particle is non-local, not necessarily in quantum mechanics.

3.2 No-path condition : uncertainty relation

We thus give up the idea of explaining the double slit experiment assuming non-locality of electron dynamics. We are then left with no option but to agree with the observation that an electron travels through both the slits at once. This tells us that the answer to the question we started with is firmly in the negative : an electron does not have a definite differentiable path. A single electron can move on two different paths at once! In the classical world we we live, this is totally weird and contrary to experience, but it seems to make sense in the quantum world.

These conclusions apply not only to electrons but to all quantum particles. The double slit experiment has been carried out with photons, neutrons, atoms, macromolecules like C_{70}, popularly known as buckey balls and even with structures as large as Bose-Einstein condensates [3, 4, 5, 6] with the appearance of the interference pattern whenever both the slits are open.

As we have seen before, lack of a definite and differentiable path for the electron implies that both the position and the momentum of the electron cannot be specified with arbitrary accuracy at the same time. This is consistent with Heisenberg uncertainty principle, which requires

$$\Delta x \Delta p_x \geq \hbar/2 \tag{3}$$

where Δx and Δp_x are standard deviations defined in Eq.(2). We will include a detailed discussion on the uncertainty principle in a later write-up.

3.3 Quantum explanation

Our next task is to develop a model which reproduces the observed interference pattern in the double slit experiment. We will have to make contact with some of the axioms of quantum mechanics.

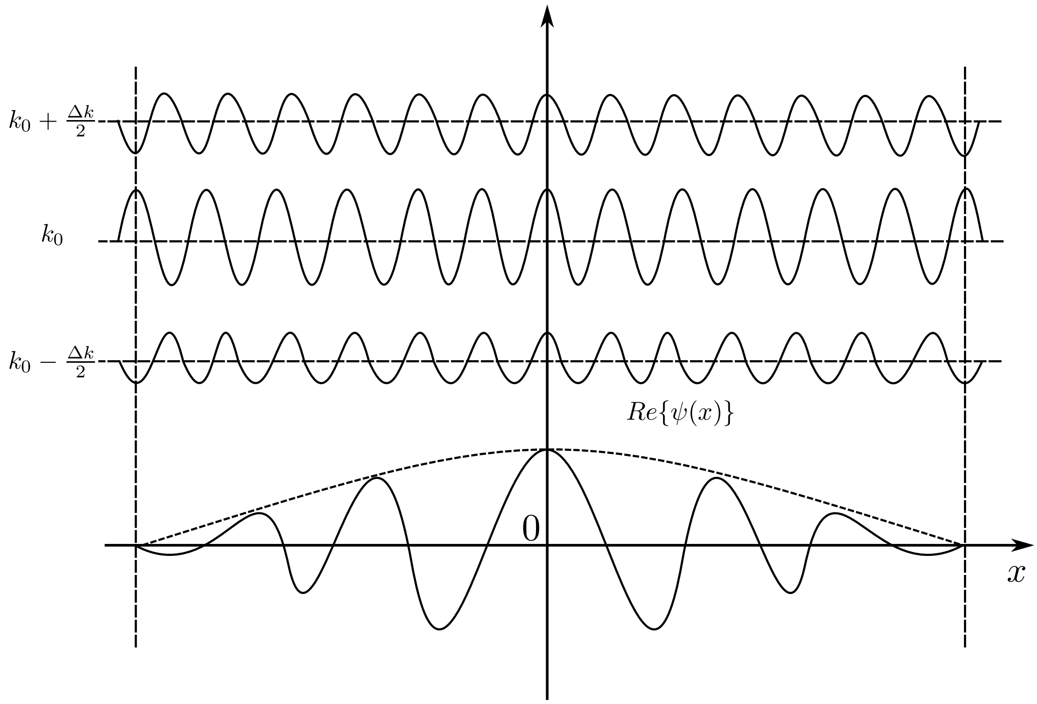

Figure 3: Superposition of waves as in Eq.4, with three values of wavenumber k_0 $k_0 \pm \frac{\Delta k}{2}$

Since the interference pattern is known to be produced by the superposition of two coherent traveling harmonic waves from two sources, we assume that the state of the electron in the double slit experiment is the superposition of two traveling harmonic waves, one from each slit. Any wave is a disturbance traveling in a medium or in free space and can be expressed as a superposition of traveling harmonic waves (see Fig.3). Restricting to $1-D$ for simplicity, a traveling harmonic wave can be represented by a complex function

$$\psi(x,t) = A\exp[i(kx - \omega t)]. \tag{4}$$

A superposition of n such waves is then a complex valued function

$$\psi(x,t) = \sum_{j=1}^{n} A_j \exp[i(k_j x - \omega_j t)] \tag{5}$$

We call this an amplitude function or a wave function. The disturbance caused by such a wave at a point x and at time t, called its intensity, is given by $|\psi(x,t)|^2$. We are interested in this amplitude function restricted to the points on the detecting screen. We denote this restriction by the amplitude function $\psi(x)$ with the position variable x on the screen. How is this wave function or amplitude function $\psi(x)$ related to the observed interference pattern on the screen? We note that $\psi(x)$ is the amplitude of the superposition of harmonic waves meeting at a point x on the screen, while our observation of the interference bands corresponds to the number of particles hitting the screen between x and $x+dx$. If we divide this number by the total number of particles hitting the screen, we get the probability of a particle hitting between x and $x+dx$. This must be the observed disturbance corresponding to the wave function defining the state of the quantum particle and equals $|\psi(x)|^2dx$. Thus $|\psi(x)|^2dx$ is the probability of finding the electron between x and $x+dx$. $|\psi(x)|^2$ is called the probability density (see footnote 2) which predicts the density of experimental points on the screen. We now free ourselves from the context of the double slit experiment and say that in all situations, a possible state of a quantum system is given by a wave function or amplitude function $\psi(x)$ or $\psi(x,t)$ if the state is changing with time. $\psi(x)$ is the amplitude of finding the particle between x and $x+dx$. The corresponding probability of finding the particle between x and $x+dx$ is $|\psi(x)|^2dx$. In $3-D$ $\psi(\mathbf{x})$ is a complex valued function of a vector argument $\mathbf{x}$ and $|\psi(\mathbf{x})|^2d^3x$ is the probability of finding the particle in the box $dxdydz$ centered at $\mathbf{x}$. We will say more about this generalization in the next section.

The traveling wave in Eq.(4) becomes intuitively more appealing when we recast it in terms of wavelength λ and period T of the wave. To get there, first we freeze the wave at some instant of time say $t=0$, so that its wave function becomes

$$\psi(x,t=0)=A\exp(ikx).$$

At the origin $\psi(0)=A$. We want to find distance λ such that $\psi(\lambda)=A$. For this we need $\exp(ik\lambda)=1$ or $k\lambda=2\pi$ or

$$k=\frac{2\pi}{\lambda}. \tag{6}$$

Similarly, $\psi(0,t)=A\exp(-i\omega t)$ giving $\psi(0,0)=A$. To get the period, we want $\psi(0,T)=A$ or $\exp(-i\omega T)=1$ or $\omega T=2\pi$ or

$$\omega=\frac{2\pi}{T}. \tag{7}$$

Thus we get the alternative form of the traveling harmonic wave

$$\psi=A\exp\left[2\pi i\left(\frac{x}{\lambda}-\frac{t}{T}\right)\right]. \tag{8}$$

Let us now try and understand how the superposition of two traveling harmonic waves produces the observed interference pattern. The wave function at some point P on the screen is given by the superposition

$$\psi(P)=\psi_1+\psi_2, \tag{9}$$

where

$$\begin{aligned}\psi_1 &= A_1\exp\left[2\pi i\left(\frac{x_1}{\lambda}-\frac{t}{T}\right)\right]\\ \psi_2 &= A_2\exp\left[2\pi i\left(\frac{x_2}{\lambda}-\frac{t}{T}\right)\right].\end{aligned} \tag{10}$$

Here A_1, A_2 are the amplitudes of the two waves and x_1, x_2 are the distances of point P from slit S_1 and slit S_2 respectively. Each term on the RHS in Eq.(9) has the same time dependence, which can be taken common, so that

$$\psi(P) = \exp\left[\frac{2\pi i t}{T}\right]\left[A_1 \exp(i\theta_1) + A_2 \exp(i\theta_2)\right] \tag{11}$$

Thus the probability of finding the particle at a distance $\leq dx$ from P is (check it!)

$$|\psi(P)|^2 dx = \psi^*(P)\psi(P)dx = A_1^2 + A_2^2 + 2A_1A_2\cos\left[\frac{2\pi(x_2 - x_1)}{\lambda}\right], \tag{12}$$

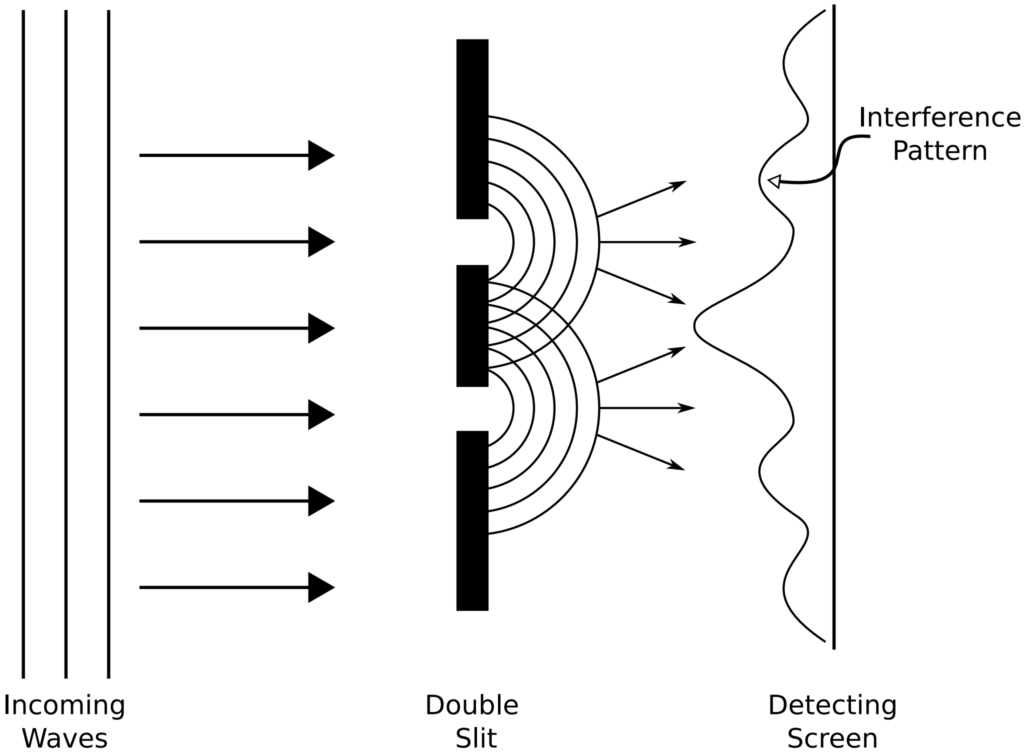

Figure 4: Two slit interference with waves(see Eq.12)

which gives the required interference pattern. A_1^2 is just what we would expect if waves were emerging from slit S_1 alone, with slit S_2 closed. Similarly A_2^2 is the term corresponding to slit S_2 open and slit S_1 closed. The last term gives the effect of the superposition of two waves. As the point P is moved up or down along the screen, this term oscillates, giving the characteristic maxima and minima of the interference pattern. All this is depicted in Fig.4.

We have already encountered one of the basic axioms of quantum mechanics, namely, the state of a quantum system is given by the amplitude function or the wave function

$\psi(x)$ and $|\psi(x)|^2dx$ gives the probability of finding the particle between x and $x+dx$. The axiomatic part of it is that this observation in the context of the double slit experiment applies to all quantum systems in all situations. This implies that the wave function of a quantum system can provide all possible information on the quantum system that we can in principle get from any experiment on the system. We will continue to explore this axiom in the next section.

We now make another contact with quantum mechanics by asking how exactly we can map Eq.(12) onto the experimentally observed interference pattern. The only undetermined parameter in Eq.(12) is the wavelength associated with the electron, namely, λ, while the electron passing through the slits is characterized by its momentum, obtained from its source parameters. So to get the wavelength associated with the electron we must connect it with its momentum. A relation between the wavelength associated with a quantum particle and its momentum was first proposed by De Broglie. This relation is

$$\lambda = \frac{h}{p} \tag{13}$$

where h is the Planck constant and λ is the wavelength of the wave associated with the particle (given the name De Broglie waves) and p is the magnitude of its momentum.

When the density of hits $|\psi(x)|^2$ predicted via Eq.(12) and Eq.(13) is compared with the observed hits forming dark-bright bands in the actual experiment as well as the positions of these bands with the peaks in the plot of $|\psi(x)|^2$, the agreement turns out to be excellent. This gives us the confidence that we are on the right track.

For the zero rest mass particles like photons, the relation between its wave nature and particle nature is given by associating a frequency ν with it via the Einstein relation,

$$E = h\nu \tag{14}$$

De Broglie and Einstein relations are at the foundations of quantum mechanics.

3.4 Which path information

Previously we have discussed the situation where one of the two slits is closed. We saw that in this case the states ψ_1 and ψ_2 (corresponding to two paths) do not superpose, the particle is either in the state ψ_1 or in the state ψ_2 but not both. When both slits are open, then both ψ_1 and ψ_2 superpose, the particle is simultaneously in both the states ψ_1 and ψ_2, which is the same thing as saying that the particle passes through both the slits. Since the superposition of states $(\psi_1 + \psi_2)/\sqrt{2}$ (factor $\frac{1}{\sqrt{2}}$ will be explained later) does not realize whenever one of the slits is closed, manifestation of this superposition, namely the interference pattern also gets eliminated when one of the slits is closed. We get the same result if we put some probe behind the slit just to find out which slit the particle is going through. In this case also, the state of the particle is either ψ_1 or ψ_2 but not their superposition, so that we do not get any interference pattern on the screen.

In fact we can state quite generally that it is impossible to find out which slit the particle is going through and also get the interference pattern at once. Interference pattern is the consequence of the superposition of quantum states (each corresponding to one path) which is fundamentally a quantum phenomenon and does not have any classical analogue.

The main message of the double slit experiment with electrons as well as photons is that both light and material particles appear as waves in certain circumstances and as particles in other. These properties are dual in the sense that experimental manifestation of one eliminates that of the other. Thus whenever the wave aspect is experimentally manifested via interference, the particle aspect (which path information) is eliminated and vice a versa. This aspect of quantum systems is often referred to as the wave-particle duality. However we note that, potentially both wave and particle aspects are inseparable. In the double slit experiment the *wave aspect* manifests itself through particle's wave function, which is the *net amplitude of finding the particle* at a point on the screen. The predictions about the behavior of a quantum particle, via its wave function, can only be probabilistic.

3.5 Quantum verses classical behavior

There are three fundamental aspects of non classical behavior of quantum systems.

1. Quantum superposition : Quantum superposition of states is an utterly non-classical concept. In the double slit experiment, when both slits are open, the electron, after passing through the slits, is in the superposed state

   $$\psi = (\psi_1(x) + \psi_2(x))/\sqrt{2} \tag{15}$$

   which gives the observed interference pattern. Here $\psi_{1,2}(x)$ are states corresponding to electron's passage through slits S_1 and S_2 respectively. Since the electron is required to pass through both the slits at once in order to produce interference, the superposition in Eq.(15) means that electron is present in both the component states $\psi_1(x)$ and $\psi_2(x)$ at once. This is in stark contrast with the classical mixture of states, where the particle is exactly in one of the component states $\{S_k\}$ and never simultaneously in more than one states. The ensemble $\{S_k, p_k\}$ has to be invoked to describe the classical mixture because we do not know exactly which of the states $\{S_k\}$ the system is in and can only specify probability p_k of finding the particle in the state S_k. Thus superposition of quantum states is an utterly non-classical feature of quantum mechanics.

2. Quantum probability : There is another utterly non-classical behavior of a quantum particle that emerges out of double slit experiment. Passing through slit S_1 or slit S_2 are the two mutually exclusive alternatives for the electron, realized by closing one of the two slits. The corresponding states are the amplitudes $\psi_1(P)$

and $\psi_2(P)$ for some point P on the screen. The corresponding probabilities are $|\psi_1|^2dx$ and $|\psi_2|^2dx$ at P. When both of these mutually exclusive alternatives are available, *we have to add the amplitudes for these alternatives to get the net amplitude at* P*, that is,* $\psi(P) = (\psi_1(P) + \psi_2(P))/\sqrt{2}$ *and then get the probability as* $|\psi(P)|^2dx = |(\psi_1(P) + \psi_2(P))|^2/2dx$. In the classical world, when there are two (or more) mutually exclusive alternatives to realize an outcome, the probability of this outcome is the addition of *probabilities* of all the mutually exclusive alternatives leading to this outcome. To see the drastic difference, consider the midpoint of a dark band so that, when both the slits are open, the probability of an electron hitting the screen at that point is zero. But the probability of an electron reaching that point when only one of the mutually exclusive alternatives is available, (that is, when one of the slits is closed), is non-zero. Thus two events with non-zero probabilities combine to give an event with zero probability!

3. No classical predictability, probability is fundamental : There is another fundamental difference between the behavior of the quantum particle as against the classical particle. If we prepare a classical particle in a definite state labeled by the values of its position and momentum then by the basic tenet of classical physics stated at the beginning, the particle possesses these values which will just be revealed in any kind of measurement of these values. Therefore if we prepare a classical system in exactly the same state again and again and measure the the values of the variables defining it, every such measurement reveals the same values. On the other hand, even if we prepare the electrons identically and pass them one by one through the double slit apparatus, the points on the screen at which they fall are completely random. Identically prepared successive electrons do not have the same value of their position on the screen. Their positions on the screen are random and completely unpredictable, we can only find out their probabilities. Put more succinctly, there is no preparation of an electron state which will make all the identically prepared electrons successively hit the screen exactly at the same point. But nothing stops us from successively shooting classical particles through one of the slits such that the particles do not scatter at the slit and land at exactly the same point on the screen. Thus the position of a classical particle on the screen can be completely predictable. In a real experiment with identically prepared classical particles, the scattering with the slits may not be avoidable and the corresponding interaction is not exactly known, therefore only the probability of a classical particle landing at a point on the screen can be specified. This probability has entered the analysis due to our ignorance and is not a fundamental property of the classical system. However, probabilistic nature of the outcomes of experiments on a quantum system is its fundamental characteristic. There may be certain states of a quantum system for which outcomes of certain experiments are completely predictable (see section 4), but these are exceptions rather than the rule.

3.6 Path integral formulation

Another idea. Suppose we start piercing the screen containing slits, so that the number of apertures in it keep increasing. Therefore the number of alternative paths by which the electron can reach a point x on the detecting screen keep increasing. Each such path contributes its amplitude to the superposition which gives the net amplitude for the electron to reach x. As the density of apertures in the intermediate screen increases beyond all bounds, the intermediate screen disappears and the paths joining the electron source and the point x on the detecting screen fill all space, which is a continuum. Hence the paths and the amplitudes contributing to the superposition become uncountably many and the superposition has to be computed by integrating over all paths. We do not say anything about how to find the amplitude for individual paths. Suffice it to say that whole of quantum mechanics can be reformulated by this method called path integral formulation of quantum mechanics. If you are interested consult ref [7].

4 General scenario

Let us summarize whatever we have learnt from the double slit experiment regarding the states and the physical quantities pertaining to a quantum system.

1. We have learnt that the state of the electron is given by the wave function or the amplitude function $\psi(x)$, which specifies the amplitude of finding the particle at all positions x on the screen. If we design the slits properly and record the data with detecting screen at various distances from the slits, we get the wave function in $3-D$ giving the amplitude for finding the particle at positions in the $3-D$ space. Here the outcome of the experiment was the position of the electron. Thus we expect that the state is obtained by specifying the amplitudes of all possible outcomes of an experiment. But we expect a state of a physical system to contain all physical information that can be extracted by performing all possible experiments on the system. If we then prepare a system in a state given by its wave function $\psi(x)$, can this wave function be used to get amplitudes for various values of system's momentum? Energy? Orbital angular momentum? The answer is yes.

2. The next aspect we have learnt is the superposition of states. The superposition (such as $(\psi_1(x)+\psi_2(x))/\sqrt{2}$) of any number of valid states of a system is also a valid state of the system. In a superposition, the system is simultaneously present in each of the component states and not in only one of them as in the case of a classical mixture. What is the meaning of the coefficients such as $\frac{1}{\sqrt{2}}$ in $(\psi_1(x)+\psi_2(x))/\sqrt{2}$? We will answer this question when we learn about the scalar product of states. Mathematically, a superposition of states is a linear combination of states (their amplitude functions or whatever symbol we use to

denote them) with complex coefficients. The set of all possible states of a quantum system is closed under the linear combination of any number of its elements.

3. Now consider acquiring which path information. If we close the slit S_2, the electron is certain to go through the slit S_1 and vice versa. Let us label the path through S_1 by 0 and the path through S_2 by 1. The corresponding states are ψ_1 and ψ_2 respectively, as defined in section 3.3. We say that if the electron is in the state ψ_1 then it is certain to take path $S_1$and if it is in the state ψ_2, it is certain to take path S_2. In other words, in the state ψ_1, the which path operation is certain to take value 0 while in the state ψ_2 it is certain to take value 1. We call ψ_1 and ψ_2 eigenstates of the which path operation and $0, 1$ its eigenvalues. Note that which path operation can take only two values.

4. Taking cue from the above observation, we state here another axiom of the theory, completely corroborated by our experience with quantum systems : contrary to the classical systems, the measurable physical quantities of a quantum system may not take all real values. A physical quantity pertaining to a quantum system may take a restricted set of real values. The set of all possible values a physical quantity can take is called the set of its eigenvalues. Corresponding to every distinct eigenvalue, there is at least one state of the system such that the probability of this eigenvalue turning up on measurement of this physical quantity on this state is unity and the system continues to be in the same state just after the measurement. This state is called the eigenstate of the physical quantity belonging to the corresponding eigenvalue. In any single run of measurement of a physical quantity on an arbitrary state of the system, only one of its eigenvalues turns up and the system is found to be in the corresponding eigenstate just after the measurement. Any value outside the set of eigenvalues never shows up in any experiment, whatever may be the state of the system.

5. Finally, we have seen that an electron does not have a definite and differentiable path, or, equivalently, its position and momentum cannot have definite values in any of its states. Generalizing, we visualize that all physical quantities are partitioned into sets such that those in different sets do not simultaneously have definite values in any state. There is no measurement which can yield values of such observables [6] with arbitrary accuracy in its single run on any state of the system. Two or more observables from the same partition (as defined above) can simultaneously have definite values in some states (actually in their common eigenstates, as we shall see later). Two or more observables, which can be measured simultaneously are called compatible, as against the incompatible ones which cannot be measured simultaneously.

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[6] By an observable, we mean a measurable physical quantity like position, momentum, energy, angular momentum etc.

How do we incorporate these facts into the structure of quantum states? The principle of superposition of states, that we have learnt from the double slit experiment, gives us the first lead. We have seen that the superposition of states is their linear combination, any number of states can be superposed and every superposition of states gives a possible new state of the system. Further, we need to express an arbitrary state as the superposition of eigenstates of an observable,whose coefficients must give the amplitudes of the corresponding eigenvalues in that state. This makes the mathematical structure of the set of all possible states of a system to be that of a linear space which we call the state space. [7] Up to now we have identified the state of a system with the wave function. The wave functions we have considered are functions of the position variable $\mathbf{x}$ but we know that it can yield amplitudes for various values of any measurable physical quantity pertaining to the system. Thus, for example, knowing $\psi(\mathbf{x})$ we can obtain the corresponding amplitude function $\phi(\mathbf{p})$ giving amplitudes for the values of momentum $\mathbf{p}$. Thus we can use one of the equivalent wave functions $\psi(\mathbf{x})$, $\phi(\mathbf{p})$ or amplitude functions of other measurable quantities to specify the quantum state. It is then beneficial to use some abstract symbol say $|\rangle$, called ket, to denote a state and find ways to get to the amplitudes of various values of a given physical quantity.

The eigenvalues and eigenvectors can be incorporated by treating every measurable physical attribute of the system as a linear operator on the state space. We can then employ standard techniques to find its eigenvalues and eigenvectors (eigenstates), which satisfy the eigenvalue equation

$$A|\lambda\rangle = \lambda|\lambda\rangle \tag{16}$$

where A is the operator corresponding to a measurable quantity and $|\lambda\rangle$ is the eigenstate belonging to the eigenvalue λ. The most important of such eigenvalue equations is the one involving the Hamiltonian of the system

$$H|\psi\rangle = E|\psi\rangle \tag{17}$$

which is known as the stationary state Schroedinger equation.

It turns out that the set of eigenstates of a linear operator on the state space corresponding to an observable is a maximal linearly independent set or a basis. We immediately conclude that any arbitrary state of the system can be expressed as a superposition of the eigenstates of a linear operator, that is, eigenstates of an observable.

Since the eigenvalues are the ones that turn up in the measurement of every physical quantity, they must all be real. Therefore, the operators representing measurable physical quantities must have real eigenvalues. The class of operators satisfying this condition are called hermitian operators. The structure of hermitian operators is discussed in all the text books on quantum mechanics. However, I have included a short exposition in the next write-up.

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[7] We assume that the reader is conversant with elementary linear algebra

4.1 Scalar products : indistinguishability of states

How do we implement the principle of superposition in the state space? In order to answer this question, we need one more structure on the state space, namely, the scalar product of two states. For every ket $|x\rangle$ we define its dual called bra, which is a functional defined as

$$\langle x| : |y\rangle \in \mathscr{H} \mapsto \langle x|y\rangle \in \mathcal{C},$$

where $\mathscr{H}$ is the state space and $\mathcal{C}$ is the set of complex numbers. The complex number $\langle x|y\rangle$ is called the scalar product of $|x\rangle$ and $|y\rangle$ if it satisfies

$$\text{(i)} \quad \langle \mathrm{x}|\{\alpha|\mathrm{x}\rangle + \beta|\mathrm{z}\rangle\} = \alpha\langle \mathrm{x}|\mathrm{y}\rangle + \beta\langle \mathrm{x}|\mathrm{z}\rangle,$$

$$\text{(ii)} \quad \langle \mathrm{x}|\mathrm{y}\rangle = \langle \mathrm{y}|\mathrm{x}\rangle^*,$$

$$\text{(iii)} \quad \langle \mathrm{x}|\mathrm{x}\rangle \geq 0.$$

Here α, β are complex numbers and the superscript $*$ denotes complex conjugation. Any dual of kets in the state space of a quantum system with the above properties can be used as a scalar product on the state space. Using the above three defining properties one can easily show that

$$\{\alpha\langle x| + \beta\langle y|\}|z\rangle = \alpha^*\langle x|z\rangle + \beta^*\langle y|z\rangle$$

which says that the scalar product is anti-linear in bra. As an example, if the state space comprises square integrable[8] amplitude functions $\psi(\mathbf{x})$ then

$$\int_{all\ space} \psi_1^*(\mathbf{x})\psi_2(\mathbf{x})d^3x$$

is a valid scalar product.

Mathematically, the state space of a quantum system is required to be a Hilbert space. If the state space is finite dimensional then defining a scalar product on it makes it a Hilbert space. Infinite dimensional state space has to be a separable Hilbert space. An infinite dimensional space (with a scalar product defined on it) is a separable Hilbert space if it has a countable basis and every converging linear combination of a basis (which is a converging series in the state space) converges to an element of the state space, that is, converges to a valid quantum state of the system. Examples of infinite dimensional state spaces are the state space of a free particle spanned by plane wave states $\{A\exp(i\mathbf{p}\cdot\mathbf{x}/\hbar)\}$ and the state space of a $1-D$ harmonic oscillator spanned by its energy eigenfunctions with eigenvalues $E_n = (n+\frac{1}{2})\hbar\omega_c$; $n = 0, 1, \ldots$ There is a subtle point here. For a free particle, its momentum values form a continuum. Therefore the plane wave basis labeled

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[8] A function $\psi(\mathbf{x})$ is square integrable if $\int_{all\ space}|\psi(\mathbf{x})|^2d^3x < \infty$.

by its momentum $\mathbf{p}$ must be uncountable. Then how can this state space be a separable Hilbert space? The answer is that no measurement of momentum (or of any measurable quantity for that matter) is completely free of errors, the actual values of momentum revealed in any measurement are a discrete countable set of values, separated by an interval determined by the error in its measurement. Thus the plane waves labeled by these discrete measured values are physically relevant and form a countable basis making the state space a separable Hilbert space.

What is the interpretation of the scalar product in the context of quantum states? The scalar product is the amplitude for the indistinguishability or the overlap of two quantum states. Two distinct classical states can always be distinguished just by measuring the values of the physical quantities defining them. However, even if two quantum states say $|x\rangle, |y\rangle$ are distinct, there may be a non-zero amplitude for the possibility that any experiment (in its single run) will fail to distinguish between them. This amplitude is given by the scalar product $\langle x|y\rangle$. People express this by calling the scalar product $\langle x|y\rangle$ to be the overlap between the two states $|x\rangle$ and $|y\rangle$. If the scalar product $\langle x|y\rangle = 0$, then the states $|x\rangle, |y\rangle$ can always be distinguished. Two states satisfying $\langle x|y\rangle = 0$ are called orthogonal. Thus two orthogonal states can always be distinguished like two classical states.

Now let us recall that when we measure a physical quantity on a quantum system in its eigenstate with eigenvalue λ, the result is λ with probability unity and the system is in the same eigenstate belonging to λ just after the measurement. In order that the last requirement of the eigenstate to make sense, the eigenstate for λ cannot have any overlap with eigenstates for eigenvalues other than λ. If this overlap is not zero, then the $\lambda-$eigenstate may not always be distinguished from other eigenstates so that it will not be certain that the state just after measurement is the eigenstate for λ. Thus two eigenstates belonging to two different eigenvalues of a measurable quantity must be orthogonal. If there are two or more linearly independent states for the same eigenvalue, any linear combination of them is also an eigenstate which shows that such eigenstates may not be orthogonal. In fact the whole space spanned by the set of these linearly independent eigenstates consists of eigenstates belonging to the same eigenvalue and is called eigenspace of this eigenvalue. It is then possible to find an orthogonal basis for the eigenspace which is the set of orthogonal eigenstates belonging to the same eigenvalue. Thus eigenstates belonging to different eigenvalues have to be orthogonal while the linearly independent eigenstates for the same eigenvalue can be orthogonalized. Thus the basis formed by all the eigenstates of a measurable quantity (called its eigenbasis) is orthogonal, that is, every pair of states in it is orthogonal and hence completely distinguishable.

Let us assume that the state space is finite dimensional Hilbert space. Consider a state $|\psi\rangle$ and the eigenbasis for a measurable quantity A, $\{|k\rangle,\ k = 1, 2, \ldots, n\}$. Being a basis, the state $|\psi\rangle$ is a superposition of the basis states. Thus

$$|\psi\rangle = \sum_{k=1}^{n} c_k |k\rangle$$

We want to understand what the coefficients c_k are. We take scalar product on both sides with a basis vector $|l\rangle$. Using orthogonality of $\{|k\rangle\}$ we get

$$\langle l|k\rangle = \delta_{kl} \tag{18}$$

(δ_{kl} Kronecker delta) so that

$$\langle l|\psi\rangle = c_l \tag{19}$$

But $\langle l|\psi\rangle$ is the amplitude for the eigenstate $|l\rangle$ getting prepared due to the measurement of A on state $|\psi\rangle$ with eigenvalue l turning up as its result. Thus $c_k = \langle k|\psi\rangle$ is the amplitude for getting the kth eigenvalue as a result of measuring A on state $|\psi\rangle$. This means $|c_k|^2 = |\langle k|\psi\rangle|^2$ is the probability that kth eigenvalue turns up and the kth eigenstate $|k\rangle$ gets prepared by the measurement on state $|\psi\rangle$.

If two different superpositions of an orthogonal basis $\{|k\rangle\}$ give

$$|\psi\rangle = \sum_{k=1}^{n} a_k|k\rangle$$

and

$$|\phi\rangle = \sum_{k=1}^{n} b_k|k\rangle,$$

then by using the defining properties of the scalar product and Eq.(18) we can write

$$\langle\psi|\phi\rangle = \sum_{k=1}^{n} a_k^* b_k \tag{20}$$

and

$$\langle\psi|\psi\rangle = \sum_{k=1}^{n} |a_k|^2 \tag{21}$$

Since $|a_k|^2$ is the probability of eigenvalue k turning up and the eigenvalues exhaust all possibilities, we must have

$$\langle\psi|\psi\rangle = \sum_{k=1}^{n} |a_k|^2 = 1. \tag{22}$$

Thus a state $|\psi\rangle$ is normalized if $\langle\psi|\psi\rangle = 1$. The norm or length of ket vector $|\psi\rangle$ is

$$||\,|\psi\rangle|| = +\sqrt{\langle\psi|\psi\rangle}. \tag{23}$$

Thus norm of a normalized state is unity. Thus a state $|\psi\rangle$ has to be normalized if $|\langle k|\psi\rangle|^2$ is to be the probability that kth eigenvalue turns up. An orthogonal basis consisting of all normalized states is called an orthonormal basis. If $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthonormal states then $\frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle)$ is the normalized superposed state.

Now we are in a position to give an example of indistinguishability of two non-orthogonal states. Consider a 2 dimensional Hilbert space with $\{|0\rangle, |1\rangle\}$ as an orthonormal eigenbasis of an operator with eigenvalues $0, 1$. Consider two non-orthogonal states $|0\rangle$ and $|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Check that the overlap is $\langle 0|x\rangle = \frac{1}{\sqrt{2}}$. Now in the single run of measuring this operator, we want to ascertain whether the system is in the state $|0\rangle$ or $|x\rangle$. If eigenvalue 1 turns up, we know for sure that the system is in the state $|x\rangle$, because eigenvalue 1 will never turn up if the system is in the state $|0\rangle$. But if eigenvalue 0 turns up, we simply cannot say which state the system is in, so that the states are indistinguishable, that is, there is no sure way of distinguishing these states. The amplitude of this indistinguishability is the same as that of 1 not turning up, that is, 0 turning up for the state $|x\rangle$, which is the same as the overlap $\langle 0|x\rangle = \frac{1}{\sqrt{2}}$.

Finally, We claim that two compatible observables, say A and B must have common igenbasis. Being compatible, both A and B can be measured simultaneously, that is, via the same act of measurement. Therefore, the state produced after the simultaneous measurement of A and B must be an eigenstate of both of them. Since all eigenstates can get prepared this way, we conclude that A and B must have common eigenbasis. Denoting this eigenbasis by $\{|k\rangle\}$ we get, for an arbitrary state

$$|\psi\rangle = \sum_k C_k|k\rangle,$$

$$AB|\psi\rangle = \sum_k a_k b_k C_k|k\rangle = BA|\psi\rangle,$$

where a_k, b_k are the eigenvalues of the observables A and B respectively, in the eigenstate $|k\rangle$. Since $|\psi\rangle$ is arbitrary we get the operator equality

$$AB = BA \text{ or, } [\mathrm{A},\mathrm{B}] = \mathrm{AB} - \mathrm{BA} = 0.$$

In other words, if the observables A and B are compatible, the corresponding operators commute. Equivalently, if A and B do not commute, then they are incompatible.[9]It is also possible to prove the reverse implication, that two commuting observables have common eigenbasis and hence are compatible. However, the proof is constructive and is worthy of a separate write-up.

4.2 Plane waves

If we write the scalar product of a plane wave with itself, we get,

$$\langle\psi|\psi\rangle = |A|^2 \int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} d^3x = |A|^2 \int_{-\infty}^{\infty} d^3x \to \infty \tag{24}$$

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[9] Incompatible observables do not have common eigenbasis, but can share some eigenstates. For example, three angular momentum components L_x, L_y, L_z do not commute, so that they are incompatible, but they share zero angular momentum eigenstate.

Thus $\langle\psi|\psi\rangle$ is infinite, therefore a plane wave state cannot be normalized. Since $|\psi\rangle$ is not normalized, $|\langle x|\psi\rangle|^2 dx$ cannot be the probability of finding the particle in volume d^3x around $\mathbf{x}$. What is the physical interpretation of such a wave function then? We can check that the probability of finding the particle in a region of space with volume V *relative* to that of finding it in a unit volume, is[10]

$$\frac{|A|^2 \int_V d^3x}{|A|^2 \int_{unit\ vol} d^3x} = V.$$

Thus for a particle in a plane wave state, the relative probability of finding it in a region of finite volume V is given by this volume V. It does not matter where in space this region is. This relative probability is uniform over all space as long as the volume of the region does not change.

It is important to realize that an ideal plane wave state is not physically realizable. Note that the absolute probability of finding the particle in a plane wave state in any finite volume V, however large, is zero.

$$\frac{|A|^2 \int_V d^3x}{|A|^2 \int_{all\ space} d^3x} = 0.$$

Thus the probability of finding the particle in the plane wave state say in the solar system is zero! Obviously, such a state is not physically acceptable.

Another way to see this is to note that a particle in a plane wave state has a definite value of momentum. Suppose there is a machine to produce a particle in a plane wave state, which is installed in a hall of volume V that is, a hall of size $V^{1/3}$. The moment this machine produces such a particle, the particle is in the hall, so that its position is uncertain only by the size of the hall, that is, $V^{1/3}$. Therefore, every component of its momentum has to be uncertain by $\Delta p \approx \hbar/V^{1/3}$, contradicting the requirement that the particle has a definite value of momentum.

Thus a practical way to treat such states is by approximating them by large enough wave packets, which can be normalized to unity and come arbitrarily close to having a precise value of momentum. Thus a state that behaves as $A\exp(ip_0x/\hbar)$ over a very large region of space and tapers off to zero outside, can be normalized to unity and has a Fourier transform so sharply peaked at $p = p_0$ that momentum measurements give results physically indistinguishable from p_0. Remember that "well defined" momentum never means "mathematically exact" but only "exact to any measurable accuracy".

4.3 Schroedinger equation

Schroedinger equation is the quantum equation of motion, or the equation describing the evolution of a quantum state $|\psi(t)\rangle$, whose initial state was $|\psi(0)\rangle$, as a result of

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[10] Note that the quantity V on the RHS is the relative probability and not volume. Although it is numerically equal to the volume over which the integral is carried out, it is dimensionless.

system's interactions with other systems and fields. I emphasize that such an equation of motion is a postulate or axiom of quantum mechanics and cannot be derived from more fundamental axioms. This situation is similar to Newton's equation of motion, which is just the statement of Newton's second law of motion, having a postulatory status. Thus the job is to make Schroedinger equation plausible using wave-particle duality. This is nicely done in many text books and I do not wish to repeat it here.

5 Superpositions revisited

We end this write-up by taking a closer look at the concept of superposition of states. We shall discuss some experimental methods to verify superpositions, apart from the double slit experiment we have already discussed.

The most important fact about quantum superpositions, which is utterly non-classical, is that the superposition

$$|\psi\rangle = \sum_k c_k |\psi_k\rangle \tag{25}$$

of a set $\{|\psi_k\rangle\}$ of quantum states, c_k being arbitrary complex coefficients, is also a possible and equally admissible quantum state. Thus the superposed state $|\psi\rangle$ corresponds to some possible physical state of the system just as the component states $\{|\psi_k\rangle\}$ do. This is to be compared with the classical mixture which is by no means a new state of the classical system but merely specifies a probability distribution over a set of states.

The above meaning of quantum superposition is amply clear from our analysis of the double slit experiment. We have seen that, when both the slits are open, an individual electron cannot be described by either one of the wave functions corresponding to the passage through a particular slit, but only by a superposition of these wave functions

$$\psi(x) = (\psi_1 + \psi_2)/\sqrt{2}.$$

Thus the superposed state $\psi(x)$ is different from the component states $\psi_1(x)$ and $\psi_2(x)$, as can be seen from the fact that $\psi(x)$ produces interference while $\psi_1(x)$ and $\psi_2(x)$ do not.

As another example, suppose we can prepare a spin $\frac{1}{2}$ particle in one of the two states $|0\rangle$ (spin up) and $|1\rangle$ (spin down). Then by superposition principle, the states $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ are equally admissible quantum states and we could therefore, at least in principle, also prepare the spin $\frac{1}{2}$ particle (separately) in both these superposed states.

Thus we see that a superposition state does not simply represent a classical mixture, that is, a classical ensemble of its component states, in which a quantum system *actually* is in only one of the component states $|\psi_k\rangle$, but we do not know exactly which. Instead, each of the component quantum state is simultaneously present in the superposed quantum state. Given the state $|\psi_k\rangle$, we can construct an orthonormal basis containing $|\psi_k\rangle$. If we carry out a measurement to this basis, with the system in the state $|\psi\rangle$ given by Eq.(25), the amplitude of state $|\psi_k\rangle$ getting prepared is $\langle\psi_k|\psi\rangle$. This overlap $\langle\psi_k|\psi\rangle$ quantifies the presence of $|\psi_k\rangle$ in $|\psi\rangle$. This situation is referred to as the existence of *coherence* between the component states. To emphasize the distinction from the classical case, a quantum mechanical superposition is often referred to as a coherent superposition. Such a superposition of component states defines a new state of the system and not merely a statistical (probability) distribution over component states.

5.1 Experimental preparation of superpositions

There are two general methods to demonstrate the existence of coherent superposition and thereby to show that coherent superposition is different from the proper (classical) mixture of its component states. First is the direct preparation of a superposed state. The second method is the indirect confirmation of the presence of all components in the superposition by means of an interference experiment. The double slit experiment falls in the second category.

One instance of an experiment which directly prepares the coherent superposition of quantum states is the famous Stern-Gerlach (SG) experiment with spin $\frac{1}{2}$ particle. I assume that you have studied the theory and experimental details of this experiment. Suppose we prepare a beam of silver atoms, all in the spin up state $|0_z\rangle$ along the z axis, which is the eigenstate of z spin operator σ_z and then send this beam through the SG apparatus with magnetic field inhomogeneous along z axis. The pattern on the screen will experimentally confirm the preparation : All the atoms will deflect upwards to impinge on the upper region of the screen. However, we know that the state $|0_z\rangle$ is the superposition of spin up and spin down states, $|0_x\rangle$ and $|1_x\rangle$ along the orthogonal x axis, that is,

$$|0_z\rangle = \frac{1}{\sqrt{2}}(|0_x\rangle + |1_x\rangle) \tag{26}$$

so that the above experimental result can be viewed as confirming the preparation of this superposition. If this superposition did represent a classical ensemble of the states $|0_x\rangle$ and $|1_x\rangle$, that is, if each spin actually was in either of the two states but not both, a single spot in the center of the screen would appear, since the inhomogeneity of the magnetic field is oriented along the z axis which cannot induce any splitting of the beam of atoms. Of course, this is not the behavior that is observed in the experiment. Conversely, we may choose to rotate the direction of the magnetic field inhomogeneity to make it along x axis, Then the input beam prepared in the state $|0_z\rangle$ will be seen to split into two equal intensity beams.

Thus the superposition $\frac{1}{\sqrt{2}}(|0_x\rangle+|1_x\rangle)$ is a new physical state of individual spin, which is different from each of the component states $|0_x\rangle$ and $|1_x\rangle$. Both the components $|0_x\rangle$ and $|1_x\rangle$ are simultaneously present in the superposed state $|0_z\rangle$, each with amplitude $\frac{1}{\sqrt{2}}$. This result also shows that the superposition of quantum states does not always manifest itself in the form of interference fringes. Here the superposition is manifested via the existence of a orientation of the magnetic field inhomogeneity in the SG apparatus such that the trajectory of the atom can be predicted with certainty.

5.1.1 Interference experiments

we have already described one interference experiment to demonstrate superposition, namely, the double slit experiment. Here the result of the superposition is the spatial interference pattern recorded on the screen. The interference pattern results exclusively due to superposition of mutually orthogonal states, each corresponding to the passage of electron through slit S_1 or slit S_2. If we use a probe to find out which of these two paths is taken by the particle, the state of the particle becomes that of the detected path, resulting in the loss of superposition and the corresponding interference pattern.

Another method to establish superposition via the observation of the interference effects is given by Ramsay interferometry [8]. In this method, interference is realized via the intensity variations in time instead of in space. Suppose we have a two level atom with ground state $|g\rangle$ and an excited state $|e\rangle$. Our aim is to demonstrate the existence of the superposed state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle) \tag{27}$$

of the atom. However, we cannot directly prepare this superposed state by measuring to the $\frac{1}{\sqrt{2}}(|g\rangle \pm |e\rangle)$ basis. We are restricted to the measurements in the $(|g\rangle, |e\rangle)$ basis. Therefore, we have to take resort to an interference method to get to our goal. First we prepare the atom in its ground state $|g\rangle$ by measuring to the basis $(|g\rangle, |e\rangle)$. By applying a laser pulse of a particular duration ($\pi/2$ pulse) to the atom in its ground state $|g\rangle$ we can make the atom transit to the superposition

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|g\rangle - i|e\rangle).$$

The state then continues to evolve :

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(|g\rangle - ie^{i\phi(t)}|e\rangle).$$

where $\phi(t)$ is the phase shift induced by the unitary evolution after a time t measured from the application of the laser pulse. [11] We now wish to establish the coherent superposition in Eq.(27). To this end we apply a second laser pulse, of the same duration as the first pulse, to get

$$|\psi\rangle = \sin(\phi(t)/2)|g\rangle - \cos(\phi(t)/2)|e\rangle. \tag{28}$$

The phase shift can be changed by changing the time interval between two pulses, introducing temporal variations into the coefficients of the superposition. If we now measure

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[11] We omit the global phase factors in $|\psi(t)\rangle$.

the atom in $(|g\rangle, |e\rangle)$ basis the probabilities of finding the atom in ground or excited states explicitly depend on the value of $\phi(t)$.

On the other hand, suppose during the time between laser pulses, the state of the atom was a classical mixture of states $(|g\rangle, |e\rangle)$ instead of their coherent superposition given by Eq.(27). The classical ensemble is determined by the probability of finding the atom in $|g\rangle$ and $|e\rangle$ states. We find from Eq.(27) that these probabilities are identical and are independent of $\phi(t)$. Therefore, in the case of classical ensemble, the observed probabilities of finding the atom in $|g\rangle$ and $|e\rangle$ states will be equal at all times. Since experiment yields time dependent probabilities consistent with Eq.(28), the existence of the superposed state in Eq.(27) is confirmed.

6 Winding up

We are now at the end of the first write-up, where our aim was to learn about quantum states and their superpositions. However, our understanding of these issues is still far from complete. There are at least two situations which we will have to address.

We have seen that quantum states form a linear space which is a Hilbert space and any number of these states can be coherently superposed to get a new state in the state space. All such states which can be coherently superposed are called pure states. But now consider the following situation. N spin $\frac{1}{2}$ particles are confined to some region of space. Suppose we know that N_u of these particles are in spin up or $|0\rangle$ state while N_d particles are in the spin down or $|1\rangle$ state, with $N_u + N_d = N$. One of these particles is drawn out at random. How can you describe its state? You will have to say that :

- The particle is exactly in one of the two states $\{|0\rangle, |1\rangle\}$ and not in both, but I do not know which.
- The probability of the particle being in $|0\rangle$ state is $p_u = N_u/N$ while the probability for its state to be [12] $|1\rangle$ is $p_d = N_d/N$.

This is just the specification of a classical ensemble of pure states $\{(|0\rangle, p_u), (|1\rangle, p_d)\}$. This is a situation where the preparation procedure of the state cannot unambiguously specify the pure state in which the system is after preparation. We have classical ignorance about the pure state in which the system is prepared. The best we can do to specify a state is to use the classical ensemble over pure states. These are called mixed states. Mixed states are far more ubiquitous in nature compared to pure states, as pure states generally involve elaborate preparation procedures not available for naturally evolving quantum systems. Pure states are rare in nature, but may not be so uncommon in a laboratory.

If the quantum system of interest comprises two or more interacting parts, each part having its own state space (when considered as separate non-interacting systems), then

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[12] These are estimates for the probability which get better as N increases.

how to construct the states and the state space of the total system? This breeds very interesting constructs like entangled states and concepts like quantum correlations, with a large variety of as yet unexplored applications.

I hope to interact with you in future.

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7 Appendix A

We give here an example which vividly illustrates the central limit theorem. I have taken this example from H.B.Callen's book on thermodynamics and statistical mechanics [9].

Consider a system comprising N "elements" each of which can take a value of X in the range $-\frac{1}{2} < X < \frac{1}{2}$. The value of X for each element is a continuous random variable with a probability density that is uniform over the permitted range. The value of X for the system is the sum of the values for each of the elements. We calculate the probability density for the system for the cases $N = 1, 2, 3$. In each case, we find the standard deviation σ defined by

$$\sigma^2 = \int f(X) X^2 dX$$

where $f(X)$ is the probability density of X and where we assume (consistent with the given $f(X)$) that the average value of X is zero. In real situations, X stands for some physical quantity whose values for each element fluctuate randomly, with a given probability density function. The problem is to find the probability density function for the values of X pertaining to the whole system, which are just the sum of the values of X for each element.

We plot the probability density and the Gaussian distribution with the corresponding standard deviation for $N = 1, 2, 3$ in Fig-5. We see that even for such a small number as $N = 3$ the probability distribution $f(X)$ rapidly approaches the Gaussian form! In this example the uniform probability density of X is chosen for the ease of calculation, but *a similar approach to the Gaussian form would be obtained for any initial probability density.*

The probability density for $N = 1$ is $f_1(X) = 1$ for $-\frac{1}{2} < X < \frac{1}{2}$ and zero elsewhere. This probability density is plotted in Fig-5(a). The standard deviation is $\sigma_1 = 1/(2.\sqrt{3})$. The corresponding Gaussian

$$f_G(X) = (2\pi)^{-1/2} \sigma^{-1} \exp\left(\frac{-X^2}{2\sigma^2}\right)$$

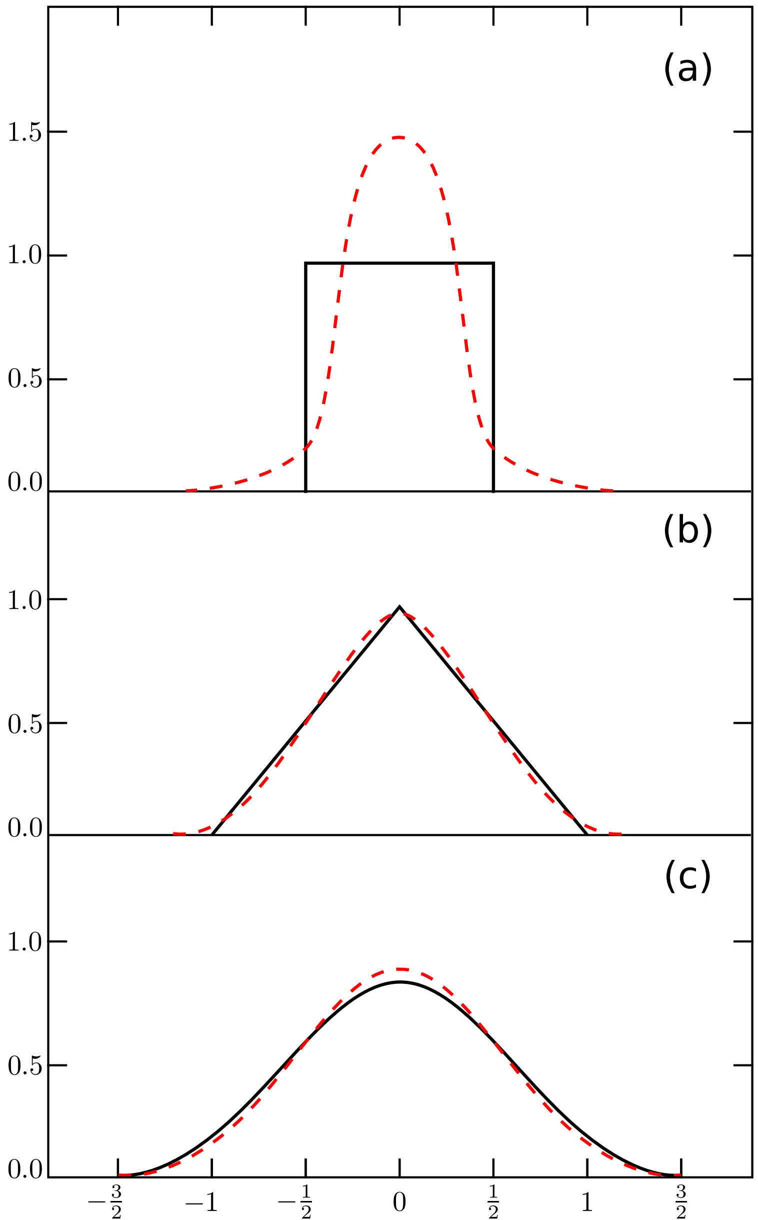

Figure 5: Convergence of probabilty density to the Gaussian form. See text.

with $\sigma = \sigma_1$ is also plotted in Fig-5(a), for comparison.

To calculate the probability density $f_2(X)$ for $N = 2$ we note (see problem A-1.1) that

$$f_{N+1}(X) = \int_{-\infty}^{\infty} f_N(X - X')f_1(X')dX',$$

or, with $f_1(X)$ as given,

$$f_{N+1}(X) = \int_{-\frac{1}{2}}^{\frac{1}{2}} f_N(X - X')dX'. \tag{29}$$

That is, $f_{N+1}(X)$ is the average value of $f_N(X')$ over the range of length unity centered at X.

We calculate

$$f_2(X) = \int_{-\frac{1}{2}}^{\frac{1}{2}} f_1(X - X')dX'.$$

X takes values consistent with $-\frac{1}{2} < X - X' < \frac{1}{2}$ and $-\frac{1}{2} < X' < \frac{1}{2}$, so that $-1 < X < +1$. For $-1 < X \leq 0$, $X - X'$ can take values on the left of $-\frac{1}{2}$ where f_1 vanishes. Therefore,

$$f_2(X) = \int_{-\frac{1}{2}}^{X+\frac{1}{2}} dX' = 1 + X \quad \text{for} \quad -1 < \mathrm{X} < 0.$$

Similarly,

$$f_2(X) = \int_{X-\frac{1}{2}}^{\frac{1}{2}} dX' = 1 - X \quad \text{for} \quad 0 \leq \mathrm{X} < 1.$$

We thus get

$$f_2(X) = \begin{cases} 1 + X & \text{if } -1 < X \leq 0 \\ 1 - X & \text{if } 0 \leq X < 1 \\ 0 & \text{elsewhere} \end{cases}$$

This $f_2(X)$ is plotted in Fig-5(b). Similarly, we find

$$f_3(X) = \begin{cases} \frac{3}{4} - X^2 & \text{if } |X| \leq \frac{1}{2} \\ \frac{9}{8} - \frac{3}{2}X + \frac{1}{2}X^2 & \text{if } \frac{1}{2} \leq |X| \leq \frac{3}{2} \\ 0 & \text{if } |X| > \frac{3}{2} \end{cases}$$

The values of σ are calculated to be $\sigma_1 = 1/\sqrt{12}$, $\sigma_2 = 1/\sqrt{6}$, $\sigma_3 = \frac{1}{2}$. Note that these values are consistent with Eq.(30). The Gaussian figures of fig-5 are calculated with these values of the standard deviations. For such a small value of N as 3, the probability distribution is very close to Gaussian, losing almost all trace of the initial shape of the single element probability distribution.

To get Eq.(29) solve the following problem.

The probability of throwing a ‘seven’ on two dice can be viewed as the sum of a) the probability of throwing a ‘one’ on the first die multiplied by the probability of throwing a ‘six’ on the second, plus b) the probability of throwing a ‘two’ on the first die multiplied by the probability of throwing a ‘five’ on the second and so forth. Explain the relationship of this observation to the expression for $f_{N+1}(X)$ in terms of $f_N(X - X')$ and $f_1(X')$ as given above and derive this relation (Eq.(29)).

To see how averaging over N values of a physical quantity x, obtained by N repetitions of its measurement under identical conditions, reduces its uncertainty or standard deviation, we make use of the following result, which we state without proof.

Let $X_1, X_2, \dots, X_N$ be N independent random variables, each having a finite variance $\sigma_k^2,\;\; k = 1, 2, \dots, N$ and zero mean. (Zero mean is not really a restriction, see below.) Define a new random variable S_N by

$$S_N = X_1 + X_2 + \cdots + X_N.$$

Then,

$$\sigma^2(S_N) = \sigma^2(X_1) + \sigma^2(X_2) + \cdots + \sigma^2(X_N).$$

In the case of interest, all $X_k,\; k = 1, 2, \dots, N$ are fluctuations around the mean which represents the 'true value' possessed by the system. All $X_k,\; k = 1, 2, \dots, N$ are identically distributed, each having the same variance σ^2, so that $X_k = X,\; k = 1, 2, \dots, N$. Further, we take mean value of this X to be zero because X and $X + C$ have the same variance for any constant C. Therefore we get,

$$\sigma^2(S_N) = N\sigma^2$$

or, in terms of standard deviation,

$$\sigma(S_N) = \sqrt{N}\sigma. \tag{30}$$

To get the value of x we must divide S_N by N so that

$$\sigma^2\left(\frac{S_N}{N}\right) = \frac{N\sigma^2}{N^2} = \frac{\sigma^2}{N}.$$

Therefore, the standard deviation, or the uncertainty in the value of x is given by

$$\sigma\left(\frac{S_N}{N}\right) = \frac{\sigma}{\sqrt{N}}.$$

We see that the uncertainty is reduced by the factor of $\frac{1}{\sqrt{N}}$ by averaging over N repetitions.

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