Spectroscopic Techniques for Pharmaceutical & Biopharmaceutical Industries

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Lecture 04~~:-~~

Introduction to Spectroscopy 4

Hello students welcome back we will continue to discuss basics of spectroscopy. So what we discussed in the last two lectures is that light can behave as both wave or~~are the~~ particle.

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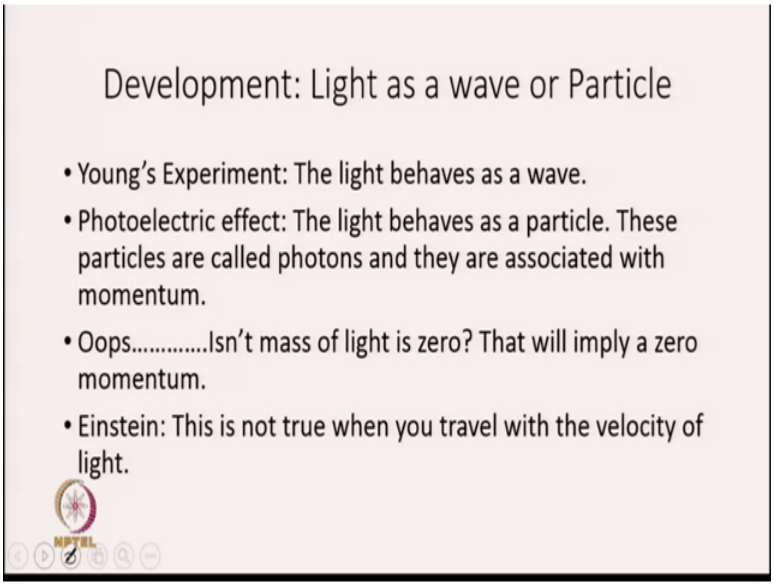

So we did see that during Young's experiment light behave as a wave so when light is passed through two pinholes a diffraction pattern was obtained which is a peculiar property of a w~~W~~ave but then during the photoelectric effect what we saw is ~~(~~light behaves as a particle~~)~~ light behaves as a particle these particles are called photons and they are associated with momentum.

Now this was a bit surprising considering that mass of light is zero what does that mean that photon should have a 0~~zero~~ momentum if photon has 0~~zero~~ momentum and how we can say it is a particle .I still explain~~ed~~ this by suggesting that momentum is not 0~~zero~~ when a particle travel with the velocity of the light.

This was very important contribution by Einstein and for that he got a Nobel Prize so Y~~J~~oung suggested that light behaves as a wave photoelectric effect showed that light can also behave as particle and Einstein~~I still~~ explained this behaviour by suggesting that a particle will not have 0~~zero~~ momentum when it travels with the velocity of light.

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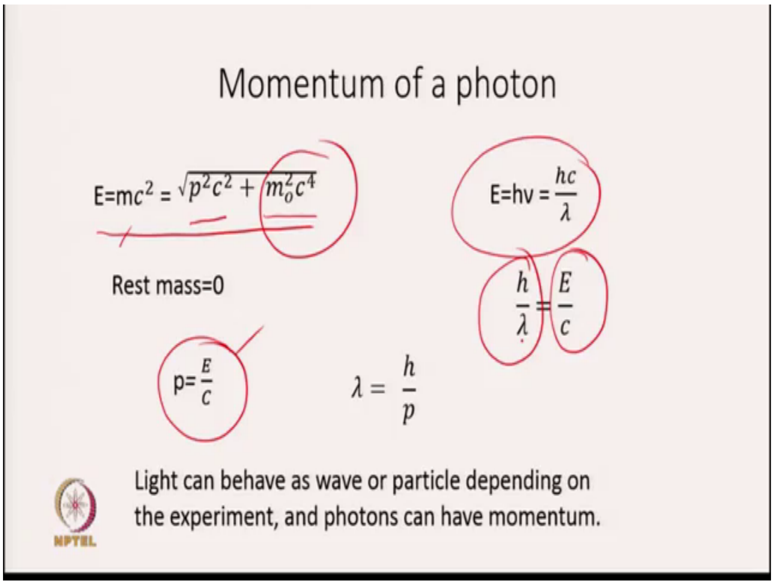

Now, let me explain this in detail, so this is the equation given by Einstein for the energy of the particle energy is given by mc~~MC~~ square and that is basically equal to a square root of p~~P~~ s~~S~~quare c~~C~~ square plus m~~M~~ not~~aught~~ square c~~C~~ 4~~for~~.

S~~ s~~o if rest mass is 0~~zero~~ that is what we expect for particles like photon then this term will be 0~~zero~~ this term will be 0~~zero~~ what does that mean is your p~~P~~ will be given by e by c~~C~~, p~~P~~ will be given by e~~a~~ by c~~C~~.

N~~ n~~ow we know that e~~E~~ is equal to hv~~HC~~ by lambda e is equal to hc~~HC~~ by lambda what does this say is that if we calculate e by c~~C~~ it will get h~~H~~ by lambda will get H by lambda and just now I showed you that p~~P~~ is equal to e by c~~C~~ and since e buy c~~C~~ is equal to h~~H~~ by lambda what does that mean is lambda is equal to h~~H~~ by p~~T~~ or p~~P~~ is equal to H by lambda so now momentum is not 0 it will be given by h~~H~~ by lambda and tha is~~t'~~s how particle and wave is correlated.

So these two ~~(~~experiments~~)~~, experiments by young an experiment done by Einstein ~~y I steam~~ which is photoelectric effect showed that light can behave as wave of particle depending on the experiments and photons can have momentum.

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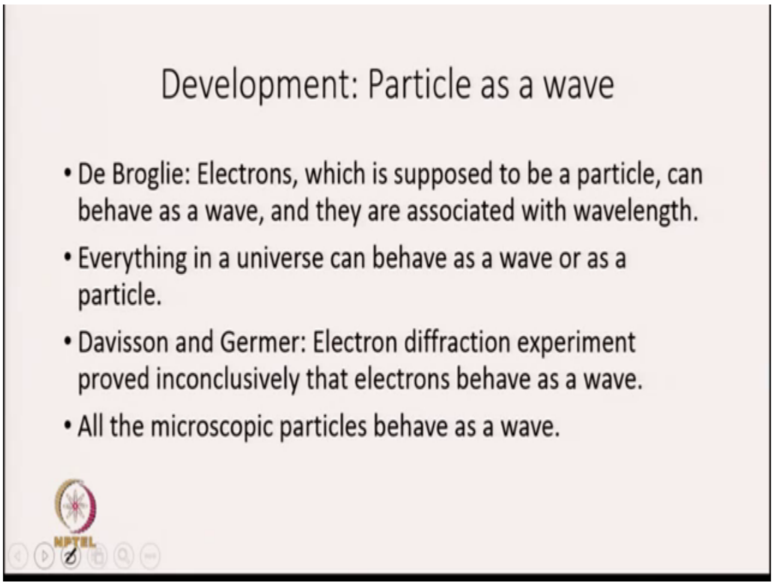

So till now we are talking about light now let us~~'s~~ see what development took place on the particle front, it was De~~deep~~ Broglie which suggested that electron which is supposed to be a particle can behave as a wave and they are associated with wavelength they are associated with wavelength.

S~~s~~o he thought that if light which a kind of wave can behave as a ~~(~~particle~~e)~~, particle also should~~ome~~ behave~~iours~~ as a wave ~~of it~~ this is basically work of his PhD theory and ~~when~~ we will surprised that de Broglie got Nobel Prize for his PhD work he also suggested that everything in universe can behave as a wave or as particle wave or as a particle and ~~they~~ this was a big statement which was proved by Davisson and Germer and ~~th~~Thomson ~~umbs~~.

W~~—w~~hat they saw that electron can behave as a wave by doing electron diffraction experiments and what does that mean is that electron apart from being a particle can behave as a wave and d~~d~~e Broglie also explained or D~~d~~e Broglie equation also suggest that all the microscopic particle can behave as a wave.

I discussed to you in the last lecture why a baseball cannot behave as a wave because wave length of a baseball with some velocity is very small very small whereas wavelength associated with electron is of the same order the size of atom size of atom and that is~~'s~~ why electrons behave~~He be~~ as a wave where as baseballs do not~~n't~~ behave as a wave~~y~~ P do not~~n'~~t behave as a wave ~~either way the~~ spin does no~~n~~'t behave as a way so these are the two important observations two important finding that both light and particle can behave as a wave and particle both can behave as wave or particle~~y~~ ~~the next important theory came about quantization of energy.~~

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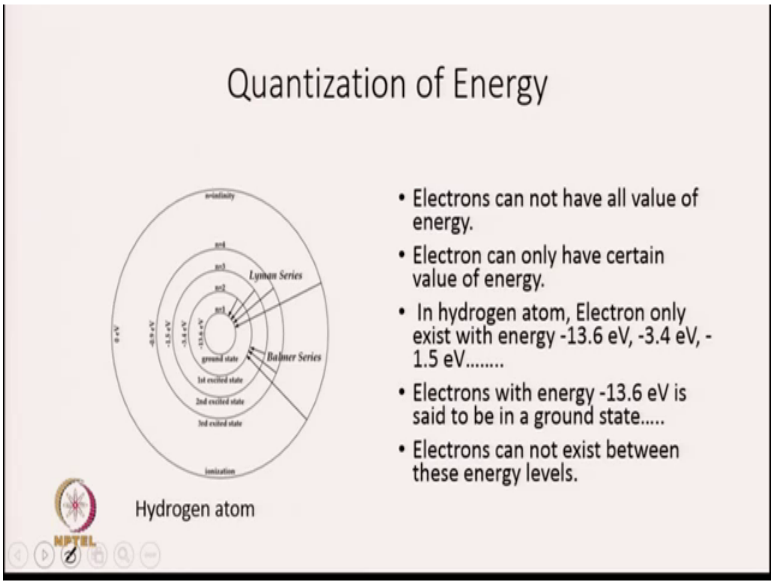

The next important theory came about quantization of energy .So, I discuss how the concept of quantization of energy came this scheme when people tried~~y~~ to explain blackbody radiation atomic spectra and heat capacity of mono atomic gas now what do we mean by quantization of energy it is very important to understand.

Q~~q~~uantization of energy means electrons cannot have all value of energy or electron can only have certain value of energy so here is a diagram of here is a electron distribution in a hydrogen atom.

~~-~~S~~s~~o now you can see that electrons can have energy minus 13.6~~thirteen point six~~ it can electrons of hydrogen can have energy minus 13.6~~thirteen point six~~ minus 3.4~~three point four~~ minus 1.5~~one point 5~~ electron volt minus 0.~~zero point~~ 9 electron volt.

S~~-s~~o in hydrogen atom electron can only exist with energy minus 13.6~~thirteen point six~~ electron volt minus 3.4~~three point 4~~ electron volt and 1.~~-point~~ 5 electron volt and so on. I~~i~~t cannot take a value between minus 13.6~~thirteen point six~~ electron volt and minus ~~three point~~ 3.4 electron volt and similarly it cannot take value between minus 3.~~three point~~ 4 electron volt and minus 1.~~one point~~ 5 electron volt.~~-so electron can have certain value of energy when~~.

So electron can have certain value of energy when e~~E~~lectron of atom of hydrogen atom has energy minus 13.6~~thirteen point six~~ electron volt it is said to be in ground state. S~~s~~o if it is here then it is said to be a ground state when it is it has energy minus 3.~~ point ~~4 electron volt it is said to be in first excited state and electron cannot exist between these energy levels so it cannot exist between minus 13.6 ~~thirteen point six ~~electron volt and minus 3.~~three point ~~4 electron volt it can be either in either have minus 13.6~~thirteen point six~~ electron volt energy or minus 3.4~~three point four~~ electron~~ight or~~ volt energy that is~~'s~~ what we mean by quantization of energy.

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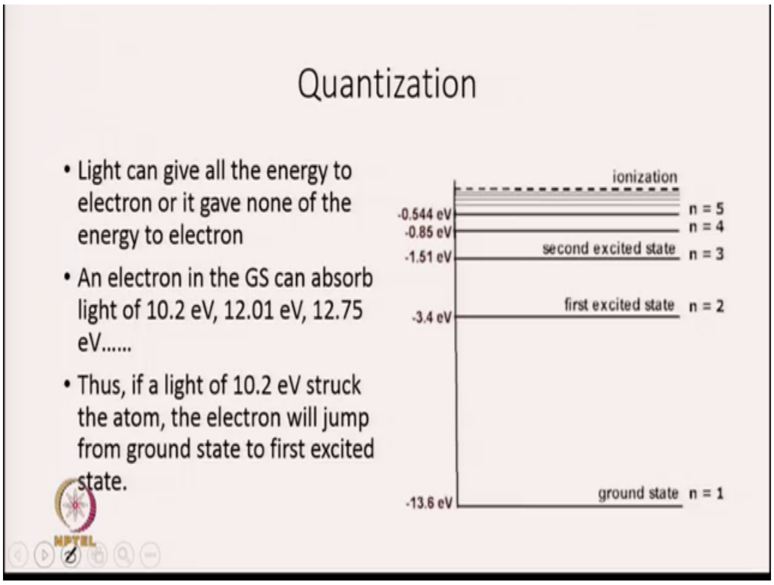

Now, what is this why this is important so suppose we bombard light on and light on a hydrogen atom light can give all the energy to electron or it gave none of the energy of electron so what does that mean so if I bombard a hydrogen atom with energy 10.2 electron volt are 12.01~~twelve point zero one~~ electron volt or~~are~~ 12.75~~twelve point seven five electron~~ volt it will absorb that energy but it will not absorb below 10.2 electron volt or suppose 11 electron volt~~eleven electron water~~.

I~~-i~~t will only absorb energy if electron if photon have energy 10.2 electron volt or ~~are~~ 12.01~~twelve point zero one~~ electron volt how does this 10.2 electron volt comes so this is the basically difference between these two energy levels.

~~-~~S~~s~~o if electron in an hydrogen atom ~~observe~~absorve 10.2 electron volt energy then it will go from ground state to first excited state ~~ground state to first excited state~~ if it absorb energy equal to 12.01~~twelve point zero one~~ electron volt then it will go to go from ground state to second excited state.

Ii~~i~~t cannot absorb energy for example here in between so they are ~~re~~ like five point one electron volt it cannot absorb that because it cannot have energy equal to minus 13.6~~thirteen point six~~ electron volt plus 5.1~~five point one~~ electron volt it cannot have that energy and that is~~'s~~ what we mean by quantization so if a light of 10.2 electron volt is struck that atom the electron will jump from ground state to first excited state.

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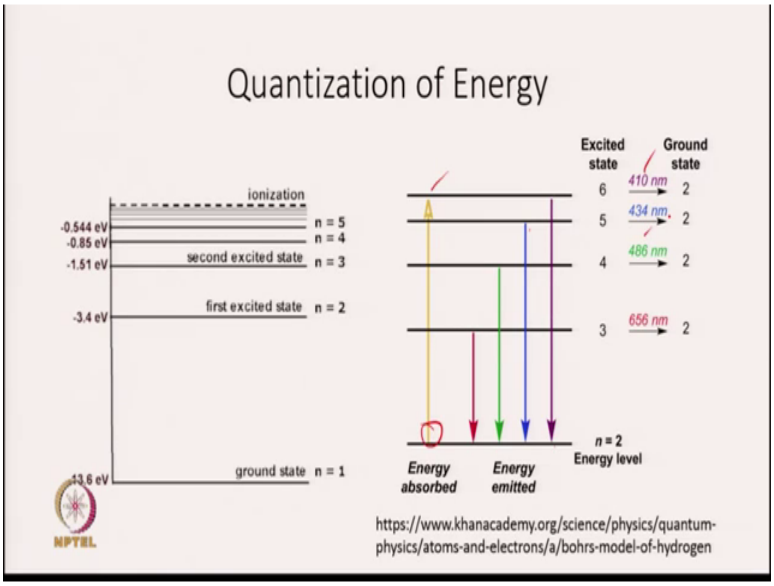

Now, let us~~'s~~ go and try to understand quantization a bit more in the last slide we did see that electron absorbs light of certain energy now what we are going to see that if it absorbs light of certain energy what can happen if it tries to meet the energy.

S ~~s~~o see here this electron takes energy and goes to suppose excited~~site a~~ state of 6~~six~~ excited state~~yesterda~~of six~~y top six~~ n is equal to 6. S~~s~~o it is going from n is equal to 2 energy level to~~2~~ n is equal to 6.

N ~~n~~ow suppose it comes back then what happens so if suppose it comes back from 6 to ground state the energy of 4-10 nanometer will be emitted or light of 410~~14~~ nanometer will be emitted if he comes back from 5 to n is equal to 2 then ~~for~~ 434 nanometer will be emitted

If~~it~~ comes from 4 to your n is equal to 2 then your 486 nanometer light will be emitted and when it comes from 3 to 2 656 nanometers light will be emitted so a ~~particel~~particulare light will be emitted what you can see here is that this all wavelength belongs to this all wavelength belongs to your visible region visible region and this is well known bomm~~b~~er series.

~~so~~So in bom~~b~~er~~s~~ is what you are doing an electron is excited from excited from level 2 n is equal to 2 to higher energy levels and when it comes back and it comes back to 2, when it comes back to energy level 2 then the light in the visible region will be absorbed ~~absurd~~ light in the visible region will be absorbed ~~observed~~.

So for absorption for going from n is equal to 2 to n is equal to 3 n is equal to 2 to n is equal to 4 a 2 to n is equal to 5 n is equal to 2 to n is equal to 6 you will need light in the visible region light in the visible region let us~~but~~ suppose you are trying to go you are trying to make an electron of hydrogen atom in the ground state to go to higher energy levels you will have to supply energy in UV region not in visible region.

~~not in visible region~~S ~~s~~o electrons from state n is equal to 1 cannot go I cannot go when electron is is in n is equal to 1 it will not absorb visible light and when it is coming back to n is equal to 1 it will again not emit light of visible region so that is what we mean by quantization of energy.

S ~~s~~o electron can only take certain value of energy and if you supply light which does not~~n't~~ corresponds to the difference between the energies which electron can take there will be no transition there can be no transition.

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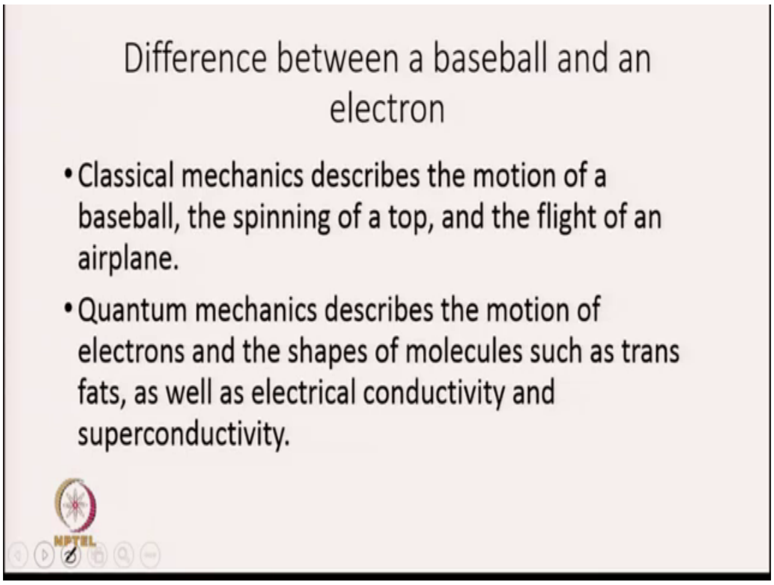

Now, there is important difference between macroscopic particle and an electron electron is a microscopic particle classical m~~M~~achanics~~kin~~ describes the motion of baseball the spinning of a top and the flight of an airplane.

S ~~s~~o I told you that baseball cannot behave as a wave and in that case it is classical mechanics which is going to describe the motion of a baseball but for particles like electrons particles like electrons which behave as a wave classical mechanics cannot describe it's motion.

T ~~t~~his quantum mechanics which will describe the motion of electrons and the shape of molecules such as transfer as well as electrical conductivity ~~in~~ and super conductivity so let us go and see how to describe motion of an electron.

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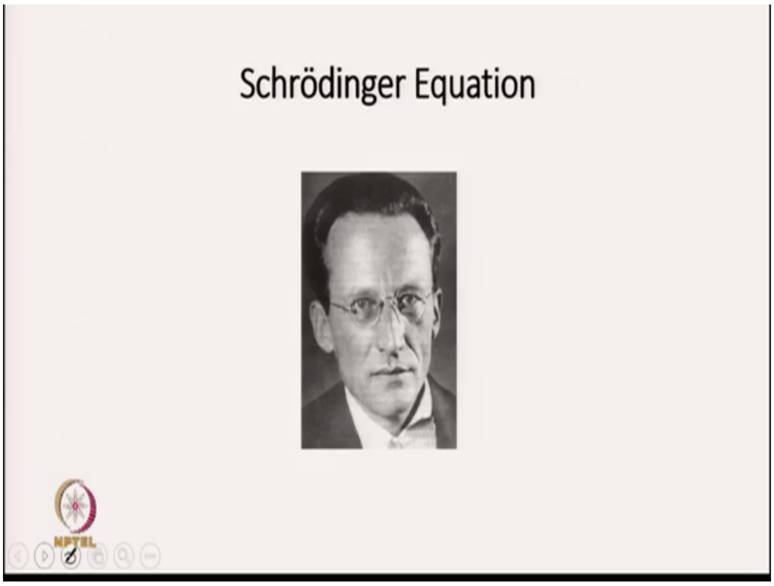

S ~~s~~o motion of an electron was described by ~~(Schrodinger equation)~~ Schrodinger equation he gave very important mathematical formulation to describe an electron trajectory. ~~an electron trajectory.~~

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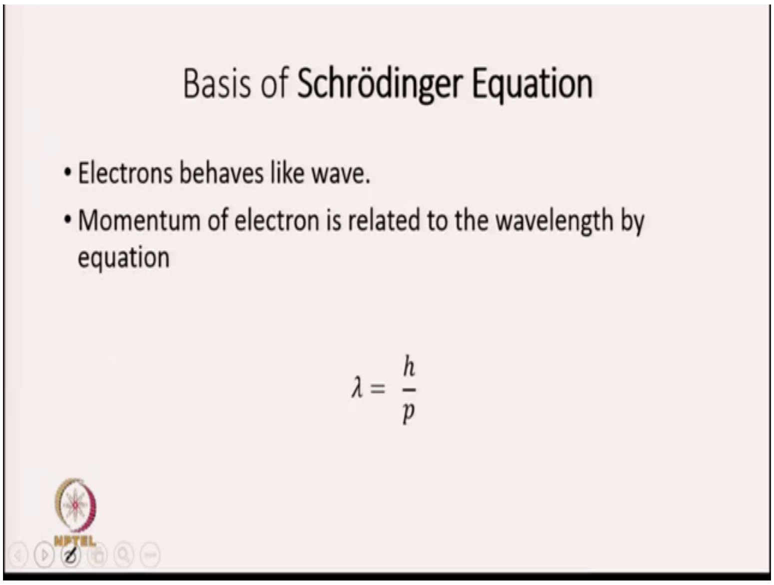

So, what is basis of his round injury question he basically was influenced by D~~d~~e Broglie he took this hypothesis that electrons behaves like a wave and momentum of electron is related to the wavelength by equation lambda is equal to H by P so since electrons behave like a wave so a wave equation~~our very question~~ can equation of a wave can describe the trajectory of electron.

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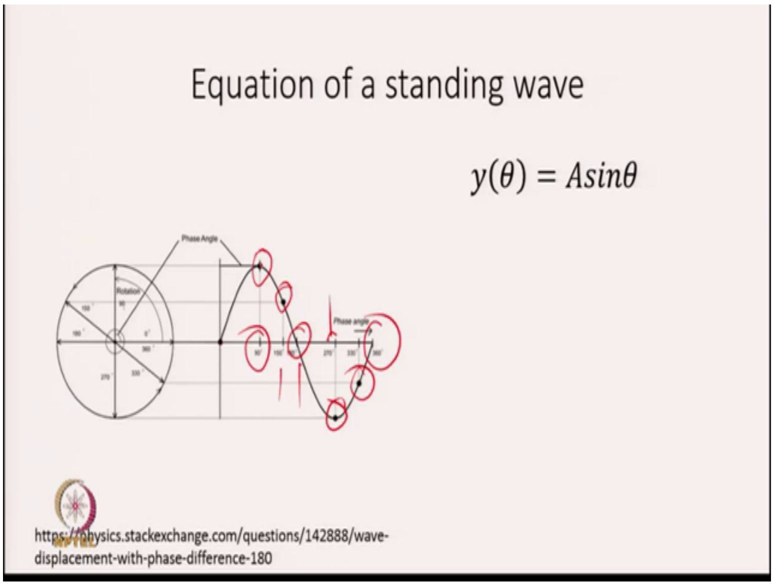

So let's think about how we can show a question of a stationary or which is not moving okay so this is your wave and I have already explained what I mean by face and this is this corresponds to zero phase this position corresponds to 90 degree phase this position corresponds to 150 degree this position corresponds to 180 degree this position corresponds to 270 degree phase and this position corresponds to 330 degree phase and this position corresponds to 360 degree phase.

S~~ s~~o what is the relation between y and this phase y~~Y~~ is basically vertical displacement so you see when theta is 0, y~~Y~~ is 0 when theta is 90 degree, your y~~Y~~ is maximum, theta is 90 degree then y~~Y~~ is maximum so this wave must be defined by the sine~~a sine~~ function.

S~~ s~~o y~~Y~~ is a~~your~~ function of this phase and that is given by a sine theta it is given by a sine theta so when theta is 0, Y is 0 when theta is 90 degree ~~-~~Y is maximum when theta is 180 then sine 1 it is 0 so again vertical displacement is 0. S~~s~~o equation of a stationary wave is function of theta and it will be given by Y theta is equal to a~~e~~ sine theta.

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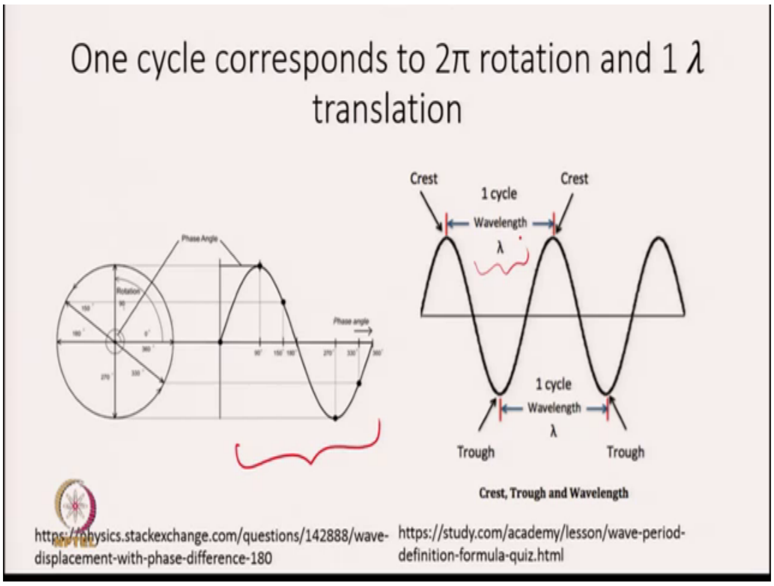

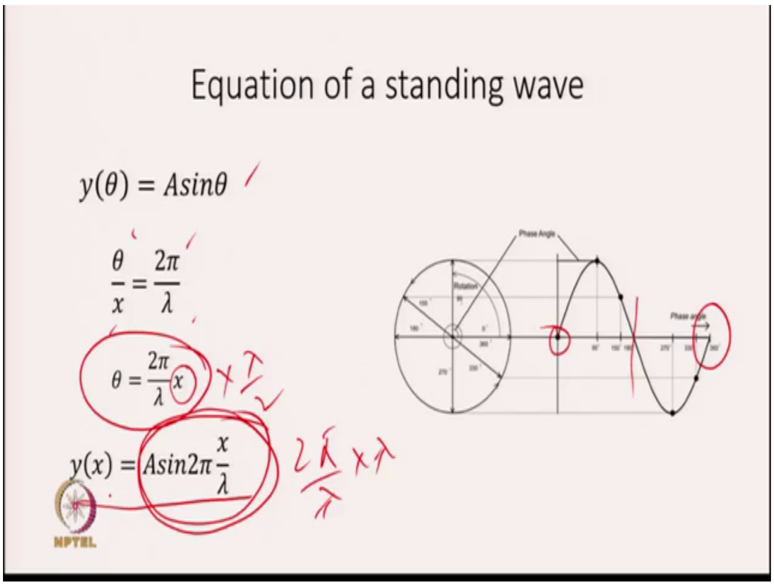

Now let's convert this this theta or try to express the equation as a function of distance so what you will see is we know that one cycle is equal to 360 degree page and we also know that one cycle the distance covered is lambda distance covered is lambda. So basically 360 degree phase is equal to one lambda

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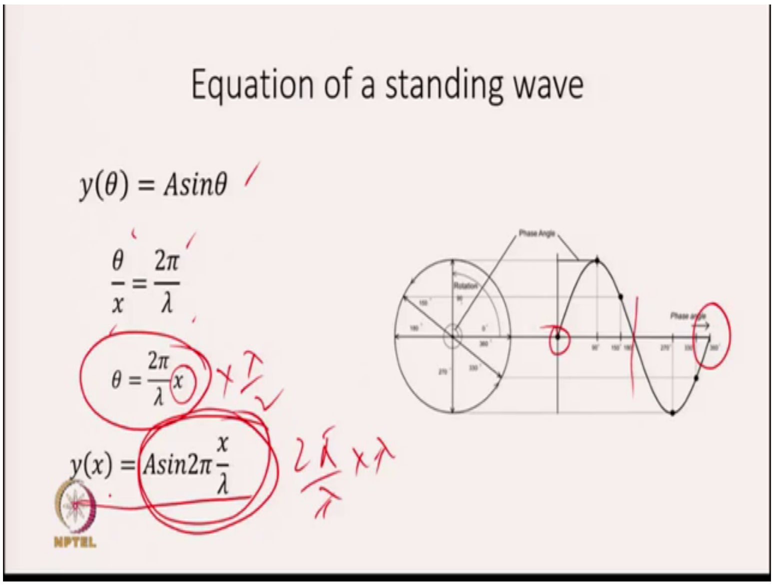

~~so basically 360 degree phase is equal to one lambda~~ so the relationship between theta and x~~X~~ which is your horizontal displacement theta by x~~X~~ is equal to 2 pie by lambda theta by x~~X~~ is equal to 2 pie divided by lambda.

S~~s~~o you can see that theta goes to 2 pie then x~~X~~ will go to lambda and theta is given by 2 pie by lambda into x~~X~~ now you can see if x is 0 theta is 0 so at this position at this point when x~~X~~ is equal to lambda by 2 if you put here then 2 pie by lambda into lambda by 2 lambda lambda ~~R~~ cancels out~~so~~ this will be pie~~PI~~ and you see 180 degree.

W ~~w~~hen x~~X~~ is equal to lambda then what will happen 2 pie by lambda into lambda so theta is equal to 2 pie ~~theta is equal to 2 pi~~ so the relation between theta and x~~X~~ is t~~T~~heta by x~~X~~ is equal to 2 pie by lambda which tells you that theta is equal to 2 pie by lambda into X and when you put in this equation when you plug in this equation what you will get is y x ~~Y X~~ is equal to a sine 2 pie x~~X~~ by lambda a sine 2 pie x~~X~~ by lambda now here you see this equation is this term is function of x~~X~~ and so now we are writing y~~Y~~ as a function of x y~~X Y~~ as a function of x~~X.~~

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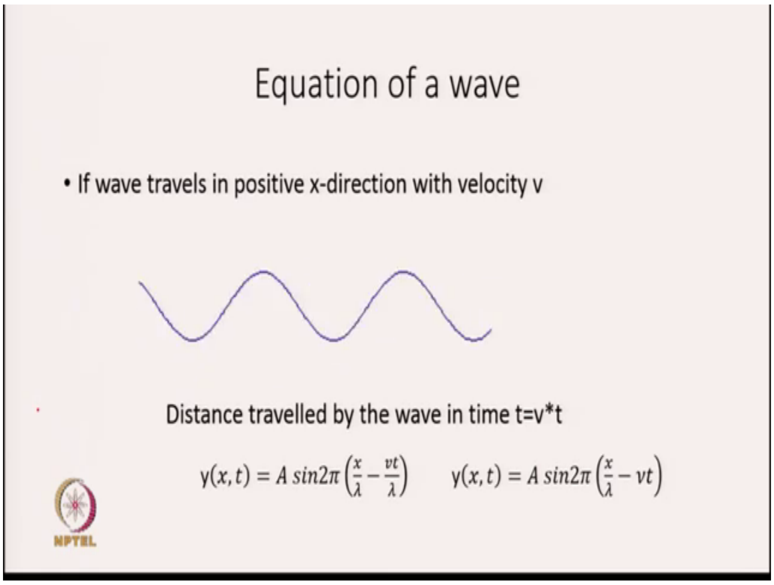

So first we described how to write y~~Y~~ as a function of theta now we describe~~d~~ how to write y~~Y~~ as a function of x~~X~~ till now we have looked at what will be the equation of wave which is standing or which is just stationary ~~Mary~~ but suppose if wave travels in positive x direction with velocity v~~V~~ then what you expect that distance travelled by the wave and the x~~X~~ direction will be v~~V~~ into T~~T V into T~~ .

I~~i~~n that case your y~~Y~~ which is vertical displacement will be given by a sine 2 pie X by lambda minus v t ~~VT~~ by lambda~~ VT by lambda~~ X by lambda minus VT by lambda ~~now~~ you see this VT velocity into time is your distance.

S~~ s~~o basically this is x~~X~~ by lambda minus another distance v t ~~VT~~ by lambda so now y~~Y~~ is a function of x~~X~~ and t~~T~~ ~~y is a function of X and T~~ and v~~V~~ by lambda is equal to frequency~~ V by lambda is equal to frequency~~ so y~~Y~~ as a function of x~~X~~ and t~~T~~ will be given by a sine 2 pie x~~X~~ by lambda minus frequency multiplied by t~~T~~ so both are x~~X~~ by lambda is unit less and frequency into time is unit less now we want to know how this vertical displacement which is y changes with x~~X~~.

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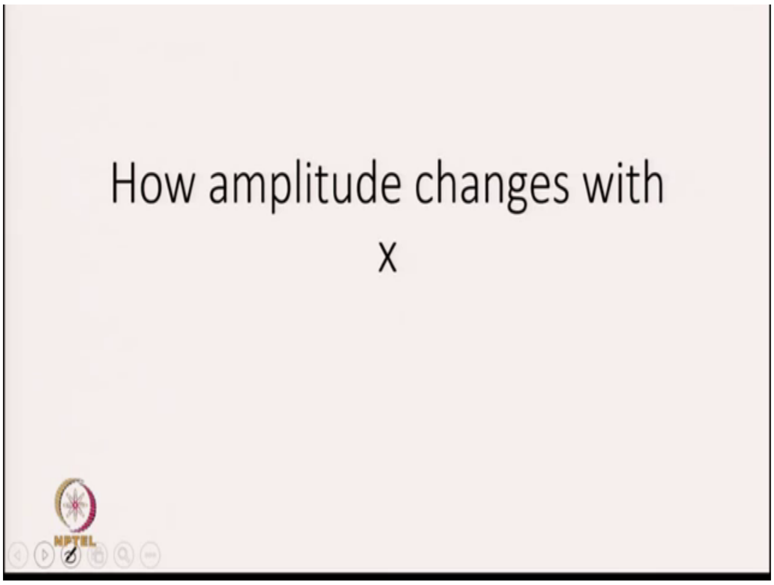

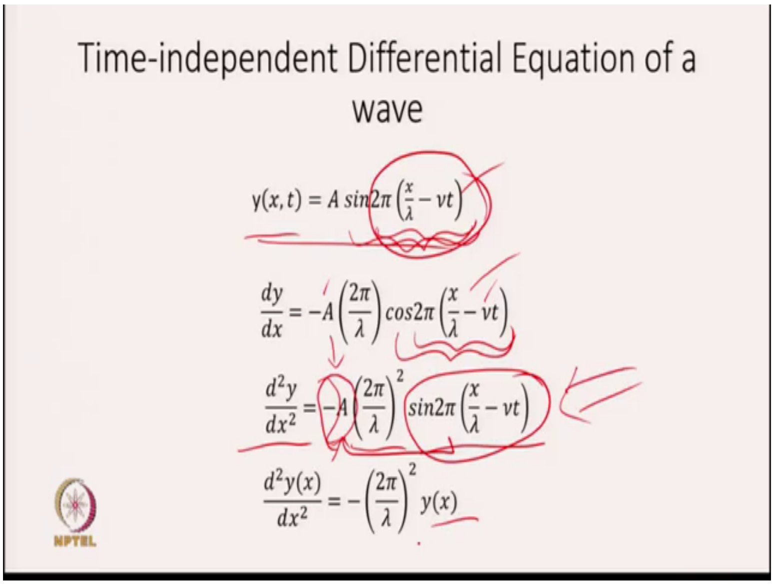

So how this amplitude changes with x~~X~~ so this is the same equation taken from earlier slide if I differentiate y~~Y~~ with respect to x~~X~~ what I am going to get is a multiplied by~~x~~ we know that differential of sine ~~X~~ x with respect to x~~X~~ will be minus cos x all right and here it is sine 2 pie x~~X~~ by lambda minus nu ~~T~~ t so what I am going to get is minus A~~a~~ into cos 2 pie x~~X~~ by lambda nu~~ew~~ t~~ea~~ frequency multiplied by time and then we need to differentiate this term which is with sign and that will be equal to 2 x by lambda since T is constant C.

~~since T is constant~~ H~~h~~ere we are assuming that it is that time is constant in that case this will not change when we differentiate with respect to x~~X~~ so minus a 2 pie by lambda so differential of this 2 pie x~~X~~ by lambda minus nu into t~~T~~ will be equal to 2 pie by lambda 2 pie by lambda okay.

I~~i~~f I differentiate again with respect to x~~X~~ what I am going to get is minus a as like this for cos I will get sine term~~urn~~ so sine term now again we have to differentiate this function 2 pie x~~X~~ by lambda minus frequency into T and then what I am going to get is 2 pie by lambda again and so this will be 2 pie by lambda square and if you look at this wave function what you will find out is that this has minus A~~a~~ term and this has this term which basically combined is equal to y x t~~Y X T~~ and you can simply write here by x in place of this multiplied by 2 pie by lambda square with minus sign.

~~with - and~~ S~~s~~o minus~~-~~ does not~~n't~~ come in here so minus sign ~~so~~ d 2 y x by d x~~DX~~ square is equal to minus 2 pie by lambda square y x~~(Y X) Y X~~ so this is time independent differential equation of a wave since we have taken t~~T~~ as a constant t~~T~~ as a constants so this is applied to any kind of wave this equation is applied to any kind of wave that means it is applied to water waves it will we applied to a sound wave and also it is applied to light wave now till this point we were not considering about we are just considering the motion of a wave.

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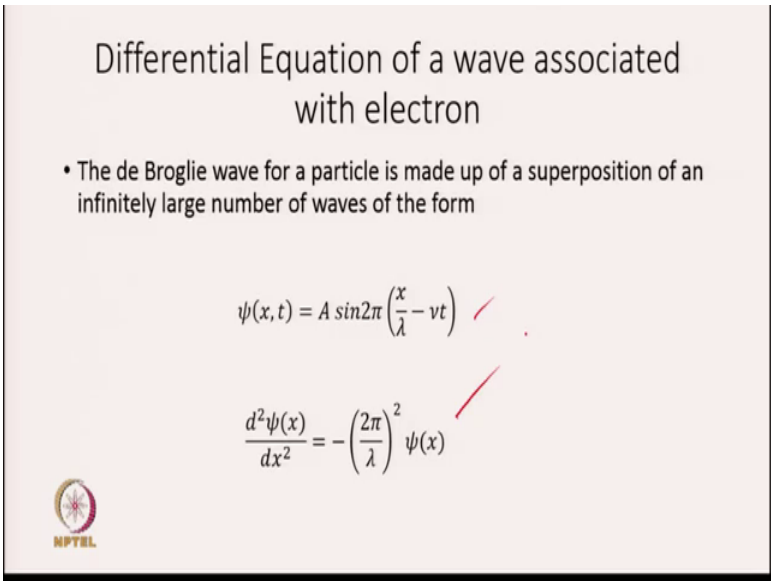

Now, let us come to see how we can write a differential equation of a wave associated with electron associated with electron so here the proposition made by De~~ded~~ Broglie comes into picture what he told that D~~d~~e Broglie wave for a particle is made up of a superposition of infinitely large number of waves of this form and for this kind of wave you have this differential equation now only thing what we have done is in place of y~~Y~~ we are now writing size~~te~~ x~~X~~ where si~~ze~~ of a function the si~~ize~~ of wave function okay so this is your wave function associated with electron.

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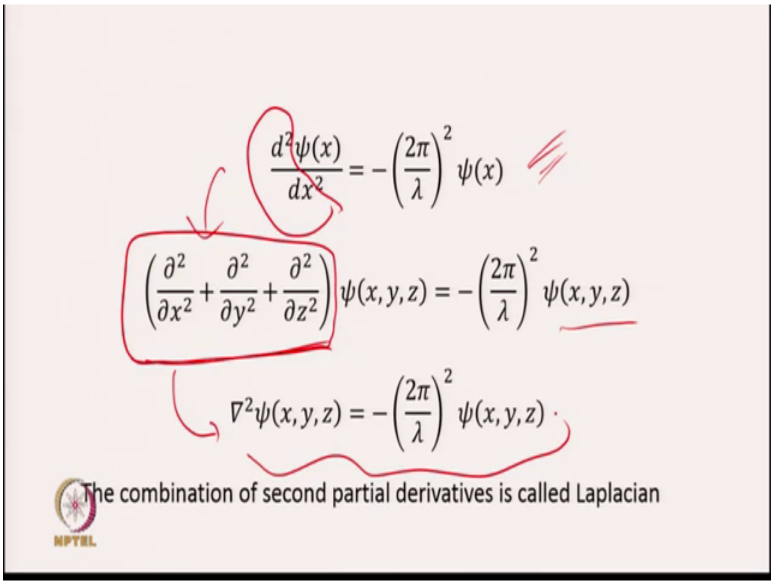

Now, what next so at this point what we are talking is one dimensional movement of the wave so this is your the equation for an electron when the wave associated with electron is moving in x~~X~~ direction but suppose if wave is moving in three dimensional space~~ three dimensional space~~ then this equation can be written like this.

S~~ s~~o now differential the double differential or second differential will be not only with respect to x~~X~~ but it will also be with respect to y~~Y~~ and with respect to z~~Z~~ so your light del square by d~~D~~el x~~X~~ square plus del square by d~~D~~el y~~Y~~ square plus del square by d~~D~~el z~~Z~~ square in place of d square by d x~~DX~~ Square and now si~~ze~~ is your function of x y z~~X Y Z~~.

S~~ s~~o same equation just only written in three dimension and to make things sort you replace this sum of three second order derivative by del s~~S~~quare and this combination of second partial derivative is known as L~~l~~aplacian so this only simplifies the thing so now this is your equation of a wave associated with electron in three dimension.

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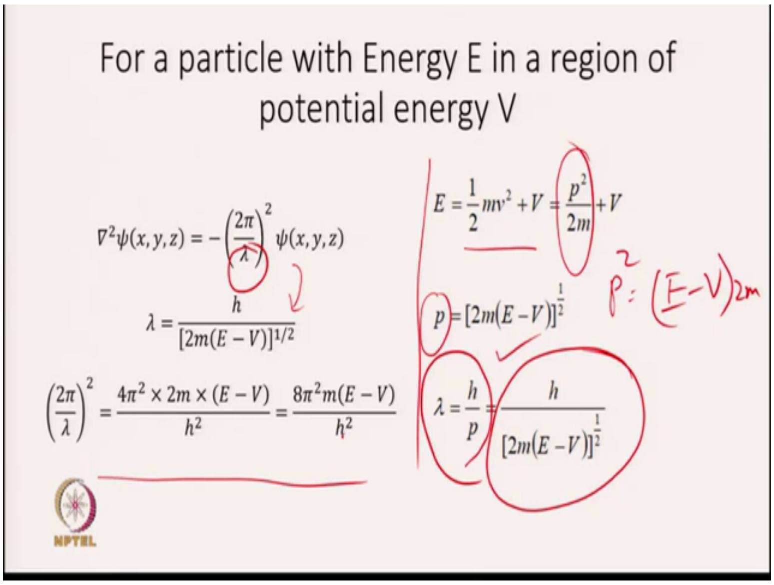

Now, what Schrodinger~~surah dinger~~ did is he replaced this lambda by h~~H~~ by p ~~P~~ so he was influenced by the hypothesis of D~~d~~e Broglie we~~'~~re deep Broglie predicted that lambda is equal to h~~H~~ by p~~P~~ so lambda associated with an electron is h~~H~~ by p~~P~~.

S ~~s~~o what can be done is just replace this lambda by h~~H~~ by p ~~P~~ so let us think so for a particle energy will be given by kinetic energy plus potential energy which is half m v~~MV~~ square plus v~~(V) V~~ is your potential energy and we know that the kinetic energy is also equal to p~~P~~ s~~S~~quare by 2 m from that you can calculate what will be the value of ~~(P)~~ p~~P~~ will be simply e p~~P~~ s~~S~~quare will be you e~~C~~ p a~~PA~~ s~~S~~quare will be e minus v~~V~~ into 2 n and so p~~P~~ is equal to 2 m e minus v~~V~~ a square root and we know that from De~~the~~ Broglie equation lambda of an electron will be given by h~~H~~ by p~~P~~.

S ~~s~~o lambda can be replaced by H by 2 m e minus v~~V~~ the square root of this so when you replace this lambda by this e~~x~~xpression what you'll get is 2 pie by lambda square will be 8 pie a square m e minus v~~V~~ by h~~H~~ square so Schrodinger took ~~your~~ equation of wave and then he plugged in value of lambda.

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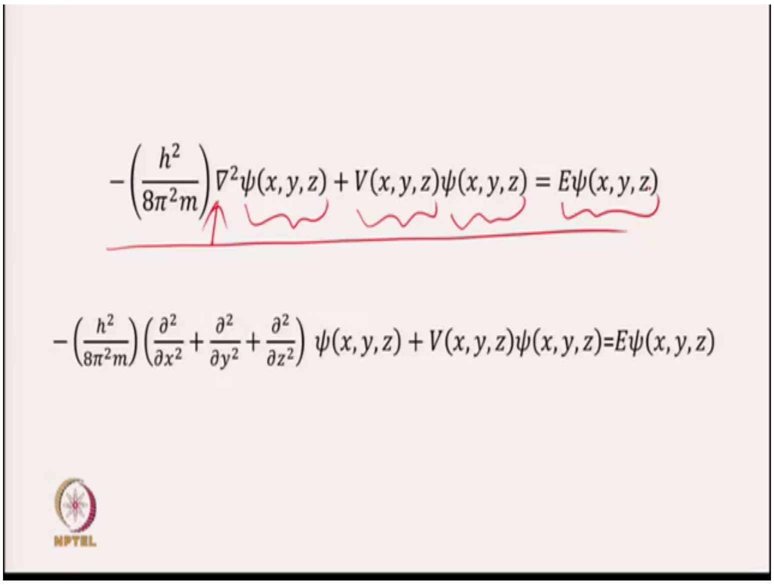

He plugged in value of lambda from D~~d~~e~~e~~ ~~broglee~~Broglie equation and what he got is well-known Schrodinger equation well-known Schrodinger equation and that is your minus h~~H~~ square by 8 pie square m the (())(34:02)~~cell depletion~~ operator into wave function plus potential energy into wave function will give you energy into wave function and this is well known Schrodinger ~~throughout dinger~~ equation. So Schrodinger utilized the concept given by de Broglie to derive equation this can tell you about trajectory of electron.

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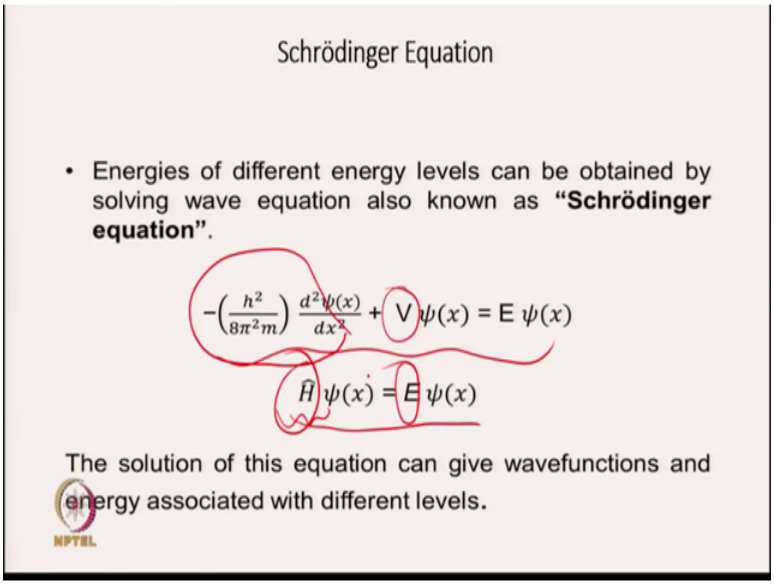

Good thing about this equation is if you solve this equation you can get the wave function and energy associated with the different quantized level. ~~energy associated with different quantized energy level~~ T~~t~~his is your Schro~~e~~dinger equation and this whole term so this is your kinetic energy term this is a potential energy term and that is given by operator h.

I~~H I~~ will just talk about operator h~~H~~ or operators what are operators but this is your equation which is known as SI is equal to e side in this equation what you are doing is you are applying Hamiltonian operator which is given by this symbol and getting your energy value getting the energy value.~~-~~so when you apply the Hamiltonian operator on the wave function what you are going to get is energy multiplied by the wave function energy multiplied by the wave function.

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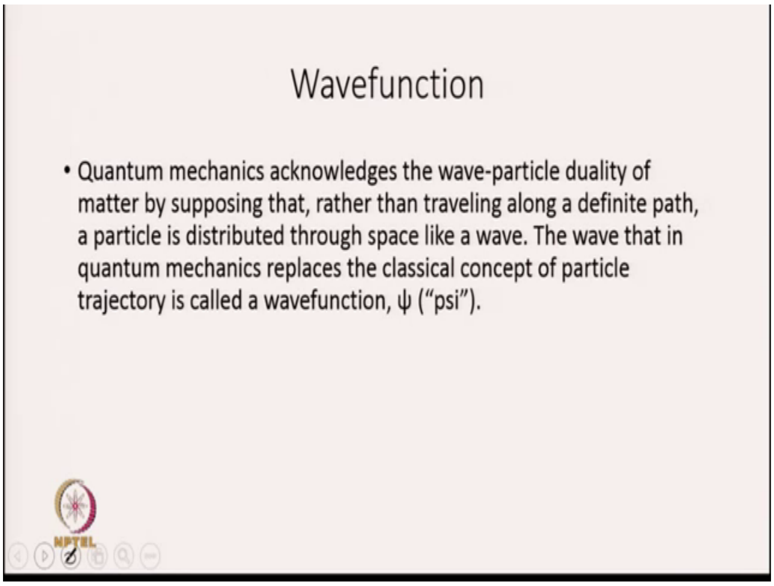

Now, there are two very important thing which comes into this Schrodinger ~~rod injure~~ equation one is wave function and another is operator in this case Hamiltonian operator so now let us discuss what are these parameters so wave function quantum mechanics acknowledges the wave particle duality of matter by supposing that rather than traveling along a definite path a particle is distributed through space like wave ~~away~~ and the wave that in quantum mechanics replaces the classical concept of particle trajectory is known as wave function so basically wave function describes the trajectory of your microscopic particles.

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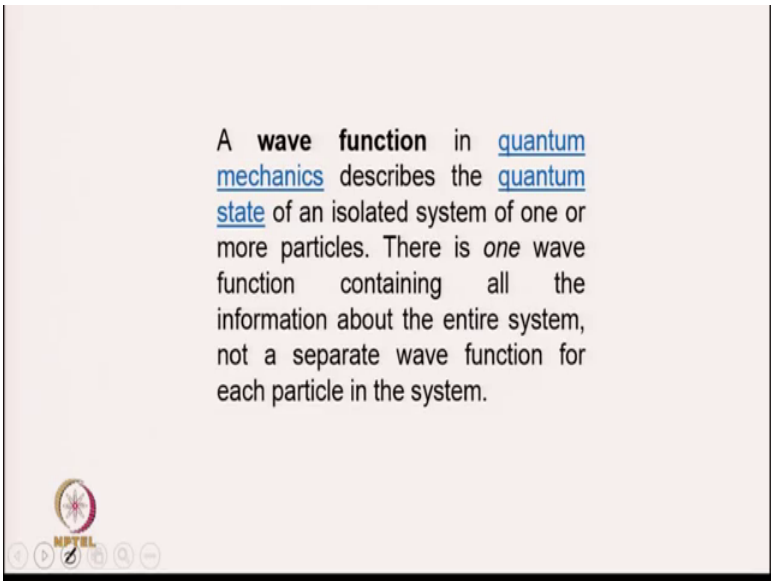

So, a wave function in quantum mechanics describes the quantum state of an isolated system of one or more particles there is one wave function containing all the information about the entire system not a separate wave function for each particle in the system that is very important part just by knowing the wave function you can tell all the information about the system all the information about the system.

~~-~~S~~s~~o what is momentum what is position what is your kinetic energy what it total energy this thing~~k~~s the information about this parameter is contained in ~~is contained~~ in the wave function.

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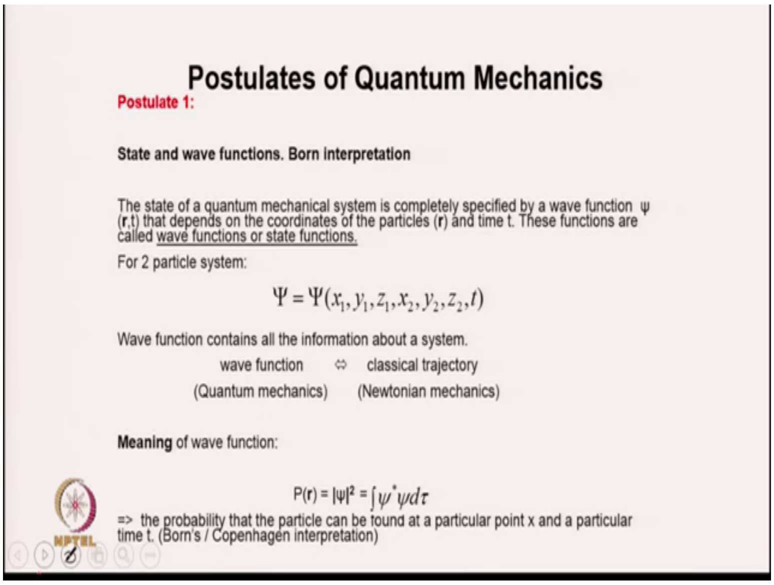

Now, let us go and try to understand wave function a bit let us~~'s~~ go and try to this~~disappoint of~~ mechanics so quantum mechanics is described by different postulates different postulate what I mean by postulate is there are certain rules have been given there are certain rules have been given and you take it as a it has face value and what it has been seen is that if you accept the postulates of quantum mechanics then the information about a microscopic particle ~~information of a microscopic particle can be obtained~~ can be obtained.

S~~s~~o first postulate is the state of a quantum mechanical system is completely specified by a wave function which depends on the coordinates of the particle and time t~~T~~ so I ha~~'~~ve already talked to you that ~~si~~psy is~~ze~~ your wave function of ~~X~~x y z~~ Y Z~~ and t~~T~~.

S~~s~~o this is for one particle system for two particle system a wave function will be a function of position of the first particle position of the second particle n type so wave function will be a function of x1 y1 z1 x2 y2 z2 and time Tt.

W~~w~~ave function contains all the information about the system and wave function is similar to classical trajectory in Newtonian mechanics wave function tells you about trajectory in the quantum mechanics what is the physical significance, physical significance is that you can get the you can find probability of particle in a~~ena~~ or around a particular point x~~X~~.~~ particular point X~~ by using this equation.

S~~s~~o probability is given by your ~~side'~~phy star into ~~sy~~psy to D tau~~D tau~~ psy~~SIA~~ star into size is known a probability density when it is multiplied by volume element and you integrate it you will get probability of finding an electron in a particular region in detail region.

S~~s~~o psy~~size~~ stars I tells you about probability density and that~~there~~ is synonymous to amplitude square amplitude square which is proportional to intensity and now you think of that what happens if volume element is small finding of an electron in ~~a~~ small volume element will be smaller.

S~~s~~o suppose in this room electron can be anywhere and suppose you choose your~~a~~ very small space in this room okay in then~~is~~ room then probability of finding electron in this volume element will be very small and in comparison to this whole~~ whole~~ room this whole room and so probability is proportional to D tau D tau is big then probability it will be ~~B~~ b and that is~~'s~~ why PR is proportional to D tau ~~P R is proportional to D tau~~ P ~~R~~ r is also proportional to psy~~size~~ star psy~~C~~ which the probability density and I explained that by giving you or by giving an analogy to~~ (intensity dependence on amplitude)~~ intensity dependence on amplitude.

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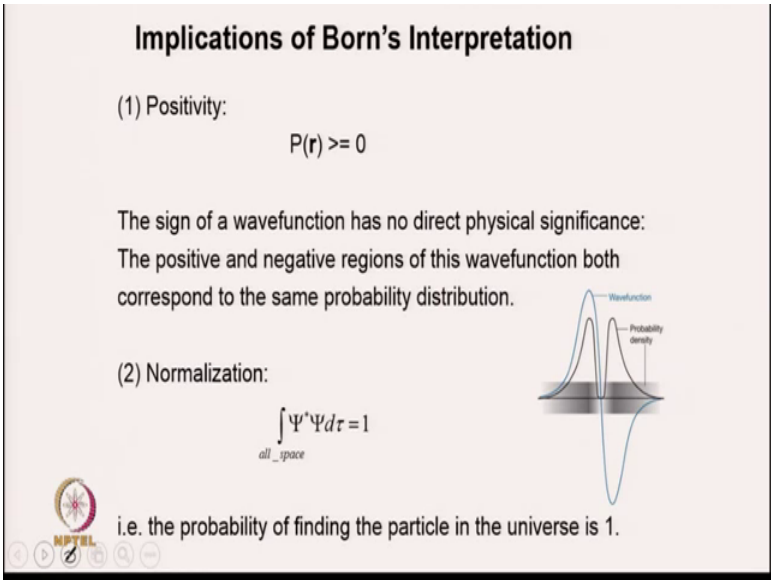

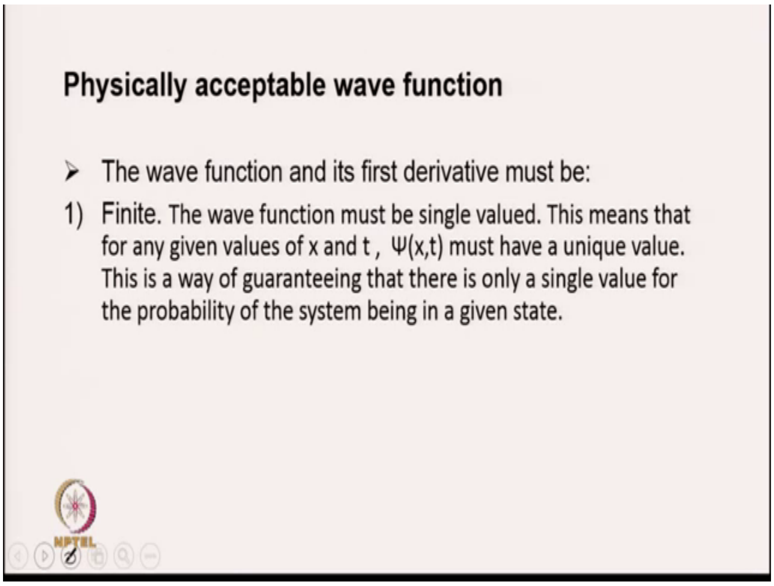

So, there are a few things which is needed your P r~~R~~ must be greater than equal to ~~zero~~ 0 here sine of wave function has no direct physical significance the positive and negative region of this wave function both correspond to same probability distribution the second thing is that that if you integrate psy~~size~~ stars psy~~sy~~ D tau over all space it should be equal to 1 and that is not a very difficult thing to understand because probability of being an electron from minus infinity to plus infinity is going to be one going to be 1.S~~ s~~ince probability of finding the particle in the inverse is 1 and that is what size should follow

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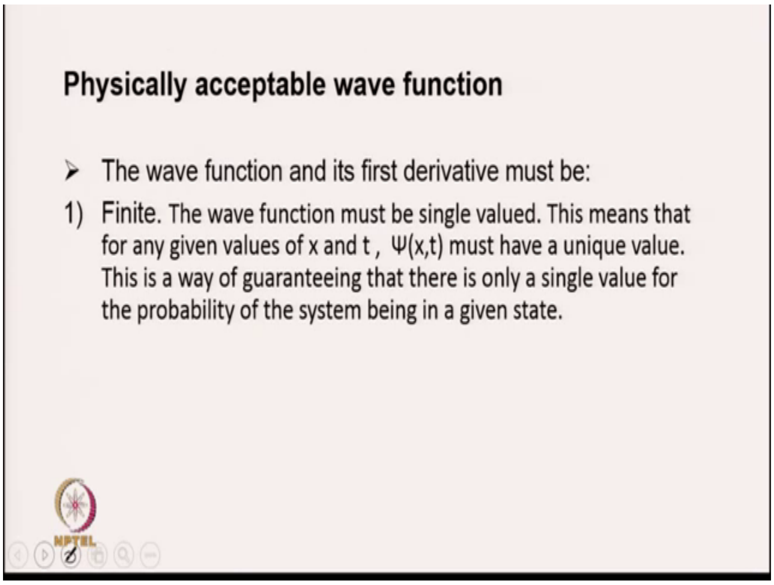

S~~s~~o there are certain rules for a acceptable wave function and that is based on the real things wave function and its first derivative must be finite or the wave function must be single valued what does that mean it means for any given value of x and t psy~~sigh~~ a wave function must have unique value and why this condition because this is way of guaranteeing that there is only a single value of probability of the system ~~(being in a given estate)~~ being in a given estate and that is quite ~~il~~logical.

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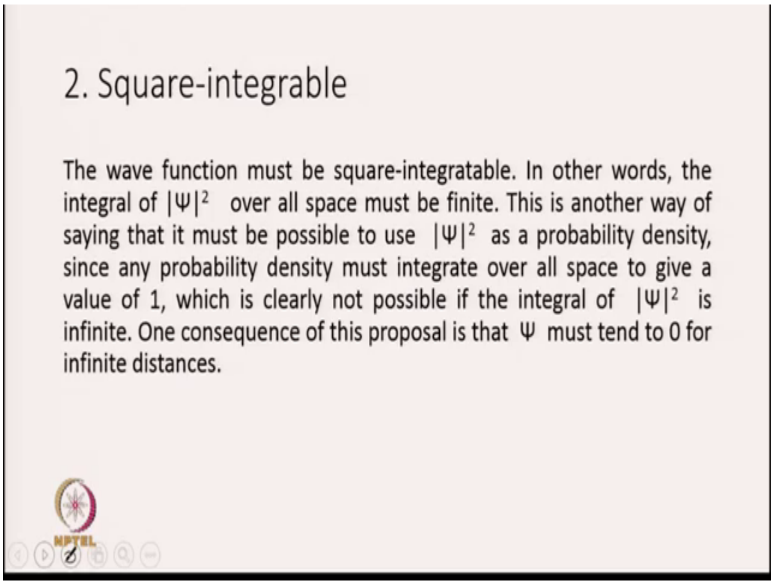

The second thing is wave function must be square integratable so what does that mean is the integral of psy~~sy~~ square over all space ~~must be finite~~ must be finite what we are telling by this is it is also logically valid because what we are trying to say by saying that function must be a square integrable is that the probability density must integrate over all space to give a value of 1 and which is not possible if the integral of Saia square is infinite and this also gives you one very important consequence that psy~~sy~~ must tends~~est~~ to zero for infinite distance ~~in finite distance.~~

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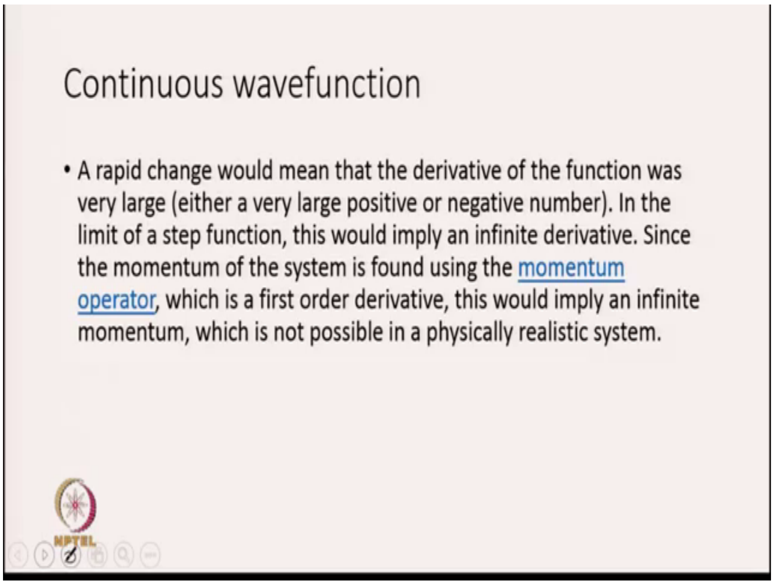

The next criteria for acceptable wave function is that wave function must be continuous a rapid change would mean that the derivative of function was very large is very large in the limit of a step function this would imply an infinite derivative later we will find out that momentum of system is calculated using momentum operator which is first order derivative and if there is a rapid change it means the derivative of the function will be very large.~~-~~I~~i~~t means in finite momentum which is not possible in a physically realistic system.~~, which is not possible in a physically realistic system.~~

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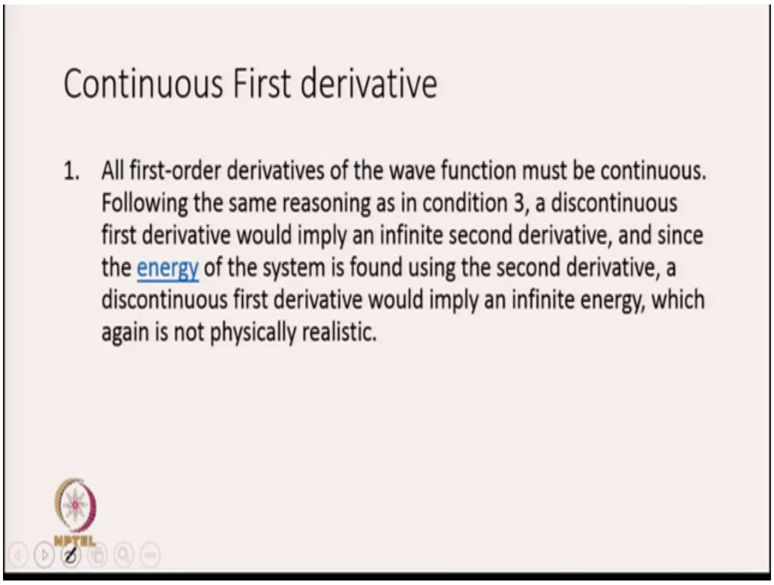

So, all first order derivative of the wave function must be continuous following the same reasoning as we did in the last ~~last~~ criteria a discontinuous first derivative would imply an infinite second derivative and generally energy of the system is calculated using second derivative so discontinuous first derivative will mean an infinite energy again which is not physically realistic.

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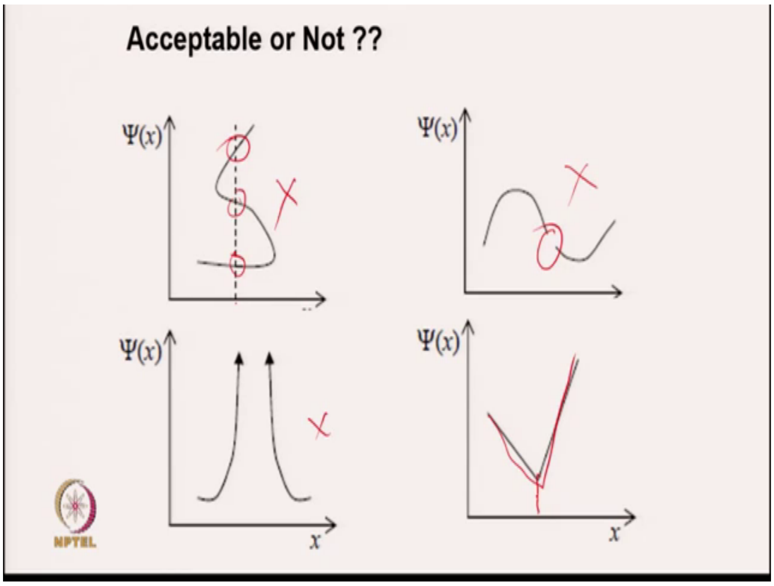

So, if you look at these wave functions this wave function is not acceptable since at this finite value of x~~X~~ you will have three different values of y~~Y~~ of size x~~X~~ so it is the wave function is not a single valued function now the second one is also not accepted because it is a discontinuous wave function third again is not acceptable and fourth is also not acceptable because you see there is a very sharp change in the wave function at this particular position of X so this wave functions are not acceptable.

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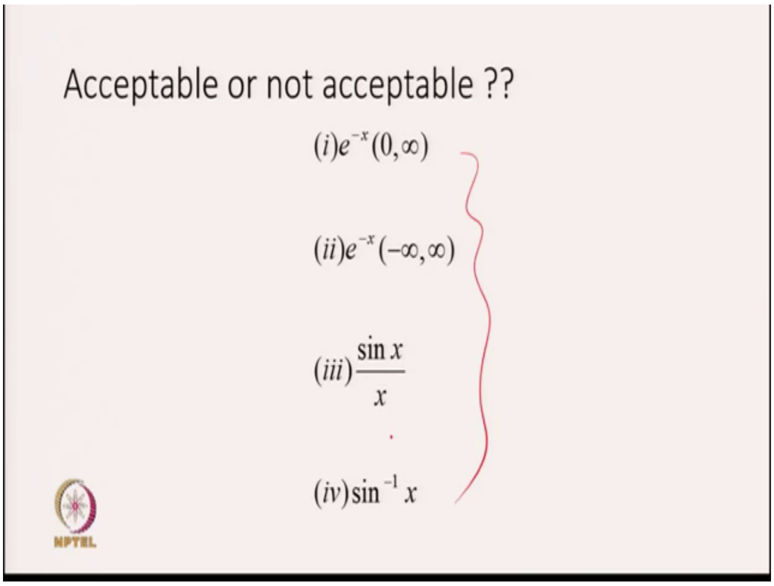

Now, let us think about this four different kind of functions exponential minus x from 0 to infinity exponential minus x~~X~~ minus infinity to infinity sine x~~X~~ by x~~X~~ and sine inverse x~~X~~.

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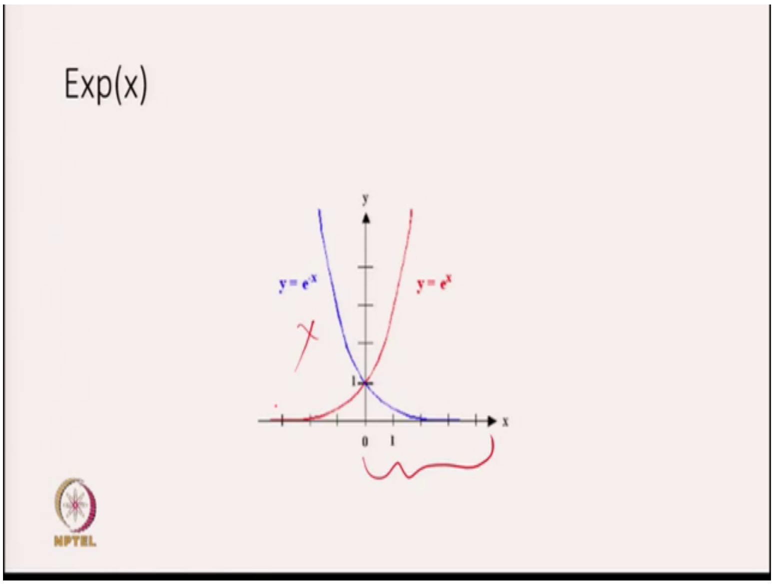

So in exponential x~~X~~ this is exponential minus x~~X~~ so you can see the plot between x~~X~~ exponential minus x~~X~~ as a function of x~~X~~ now you see here this wave function is acceptable if we take from 0 to infinity if we remain in the region 0 to infinity but this is not acceptable in a reason when you go from~~m (0 to minus infinity)~~ 0 to minus infinity.

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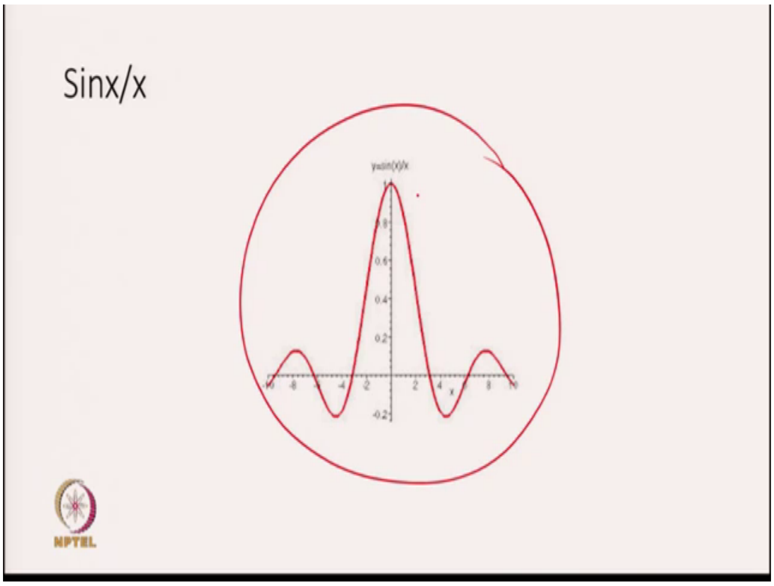

Sine ~~X~~ x by x~~X~~ this is an acceptable wave function it meets all the criteria for an acceptable wave function.

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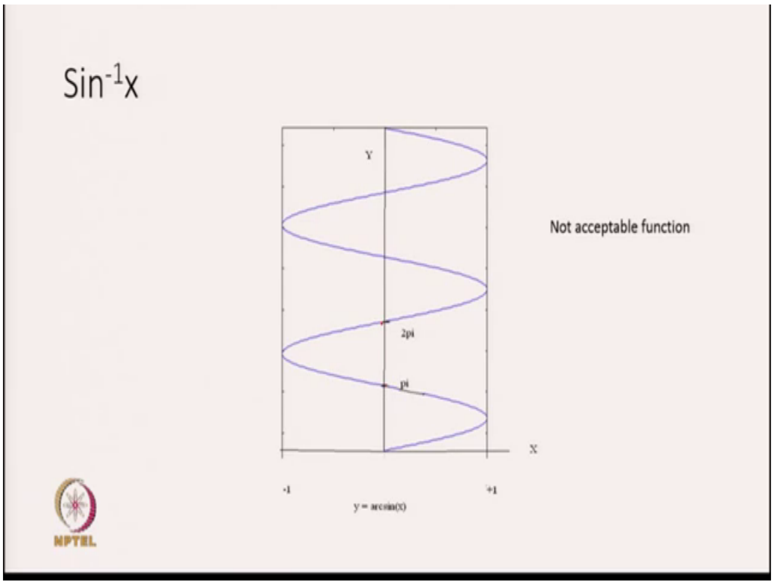

Sine inverse x~~X~~ this is the plot of sine inverse x~~X~~ versus x~~X~~ is a plot of sine inverse x~~X~~ versus x~~X~~ now you can see that x~~X~~ will be 0 at y~~Y~~ is equal to 0 y~~Y~~ is equal to pie~~PI~~ Y is equal to 2 pie and so on so this wave function is not a single valued function and so it ~~(cannot be a acceptable wave function)~~ cannot be acceptable wave function.

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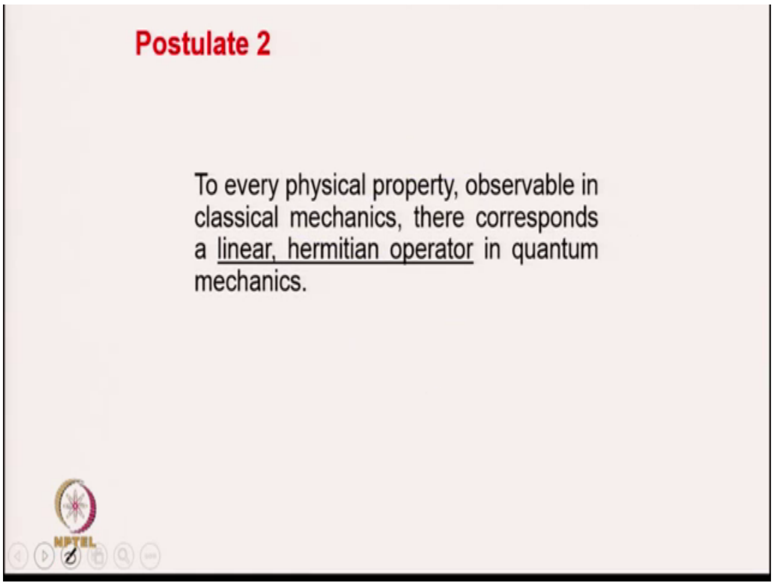

Now, a postulate 2 tells you for every physical property observables in classical mechanics there corresponds a linear hermitian operator in quantum mechanics so there are three important part of this postulate money observable what we mean by observable and then the second is operator third is your linear and fourth is hermitian so we will~~'ll~~ go to every this four of them one by one and try to understand what we mean by this.

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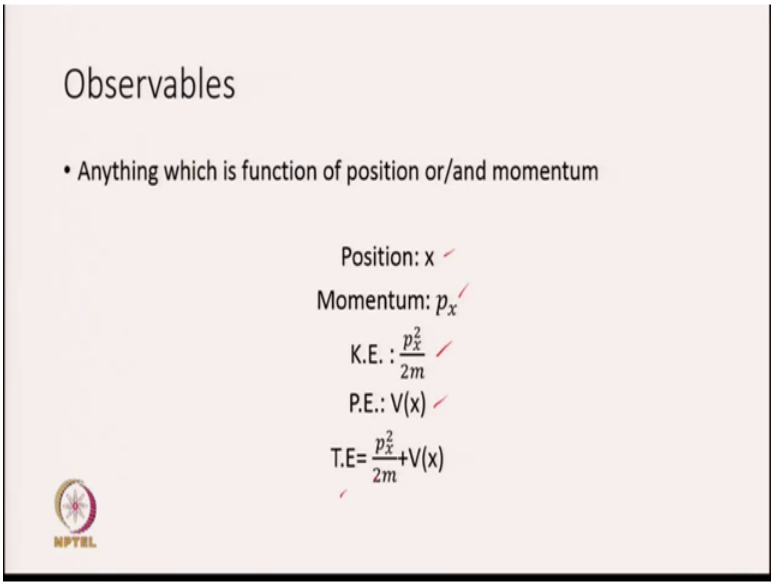
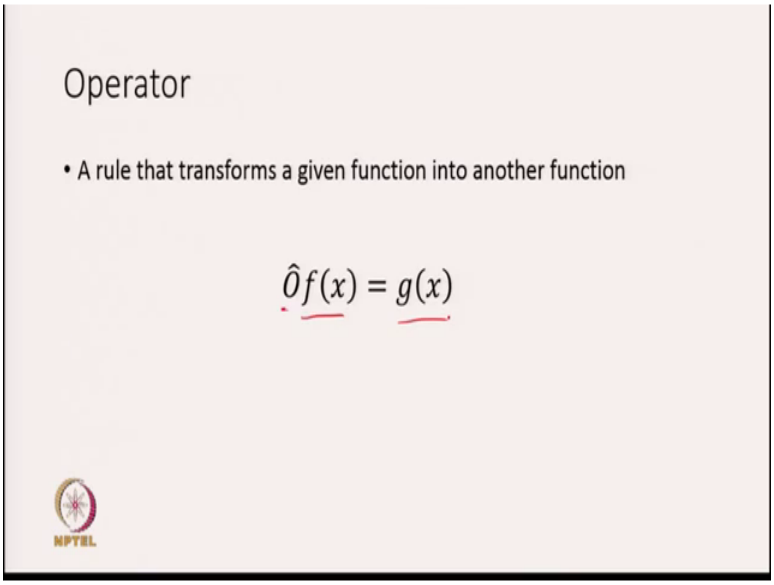


So, let's discuss about your observables what are observables, observables are anything which is a function of position or an~~d~~ momentum for example position is a function of X momentum which is function of p x~~x~~ kinetic energy which is a function of P momentum your potential energy which is a function of position and total energy which is a function of position and momentum so these are the observables.

(~~Reference~~Refer Slide Time 51:~~.~~07)



What are operators? operator is a rule that transforms a given function into another function so if you apply operator O~~o~~ on a function f x ~~FX~~ it will give you another function which is your g x~~GX~~ so operator transforms a given function into another function so here operator O~~o~~ is converting a function f x~~FX~~ into another function g x~~GX~~. ~~another function GX.~~

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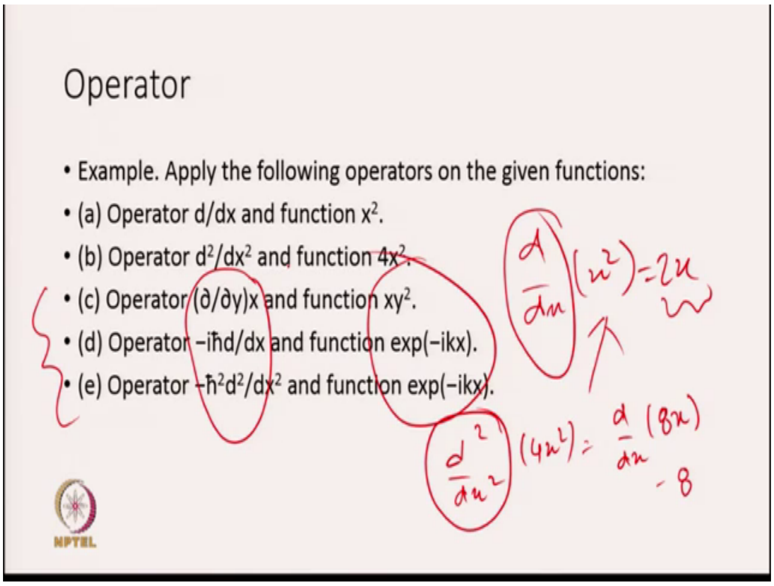

Now, let us understand by some examples so suppose either operator d~~D~~ by d x~~DX~~ when I apply that on function x~~X~~ square we will~~'ll~~ get another function 2 x d~~D~~ by d x~~DX~~ is x~~X~~ Square d~~D~~ by d x~~DX~~ x~~X~~ square is equal to 2 x.

S~~s~~o this is first function when you apply this operator d~~D~~ by d x~~DX~~ it will give another function which is equal to 2 x similarly when we apply operator d square by d x~~DX~~ square on 4 x square what we will get will get first d~~D~~ by d x~~DX~~ 8 x and then this will give you 8. ~~this will give you 8~~

S~~s~~o when we apply this operator ~~this operator~~ double differential operator on the function four x~~X~~ square we are going to get 8 similar kind of operator you can see here and you can practice what you will get when you apply these operators on these functions on these functions this is about operator part.

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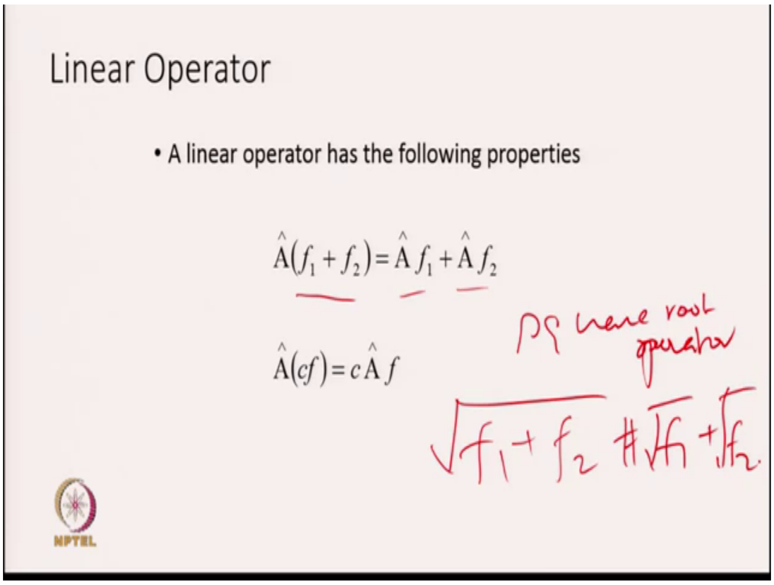

What is a linear operator a linear operator has the following property if I take a combination of two function f 1 and f 2 and if I apply a linear operator you take that value and then what you do that apply this linear operator to function f 1 and f~~F~~ 2 separately then the two values must be equal to values must be equal.

N~~n~~ow you will see that it should be equal for every operator no it is not like that for example suppose you have a square root operator~~ a square root operator operator~~ okay so a square-root operator for example this one f1 plus f2, f2 will not be equal to a square root of f 1 plus a square root of f~~F~~ 2 ~~s~~ square root of Hector.

So~~ s~~o this condition does not ~~n't~~ hold true for every operator but this will be true for a differential operator this will be true for a differential operator so differential operator is a linear operator so when operator is applied to a combination of two different function and it is equal to then apply some of your when you apply operators separately to this two function then you have a linear operator.

T~~t~~he second condition which also should be maintained is when you apply this operator to a function multiplied by a constant you must get constant multiplied by ~~x~~ operator~~ of that function constant x operator~~ of that function so two condition you apply operator to the combination of two wave functions if it is equal to operator of function f_1 plus then plus operator of function f_2 and the second is an operator is applied to a constant multiplied wave function that should be equal to constant multiplied by operator of this function.~~ ~~so we discussed observables we discussed your operator I~~D~~ discussed ~~first~~ your linear operator so now we will go to hermitian operator.

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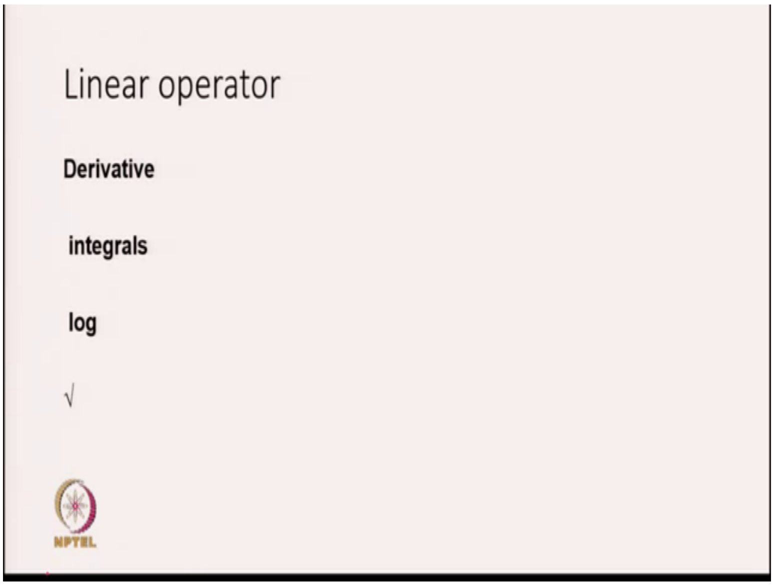

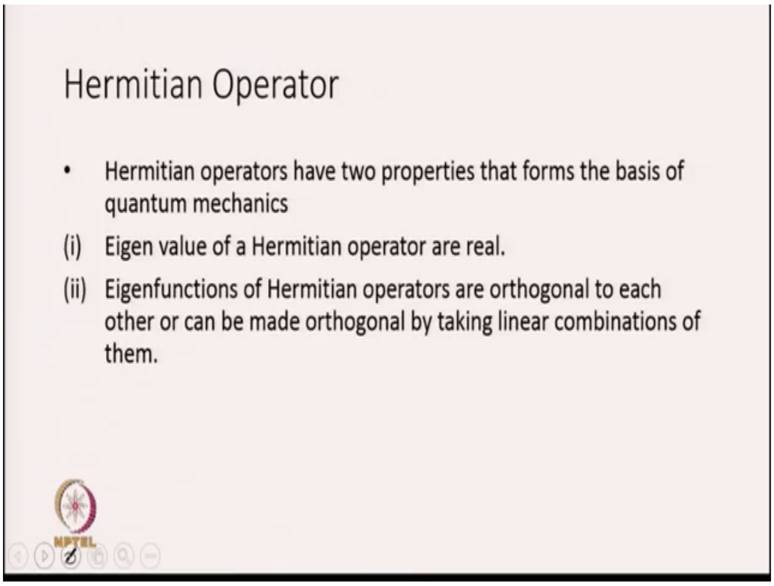

But before that I will tell you to look at these four questions to look at these operators and tell whether these operators are linear or not so check whether derivative is a linear operator where integral is a linear operator the log is a linear operator where a square root is a linear operator I just discussed about a square root it is not a linear operator.

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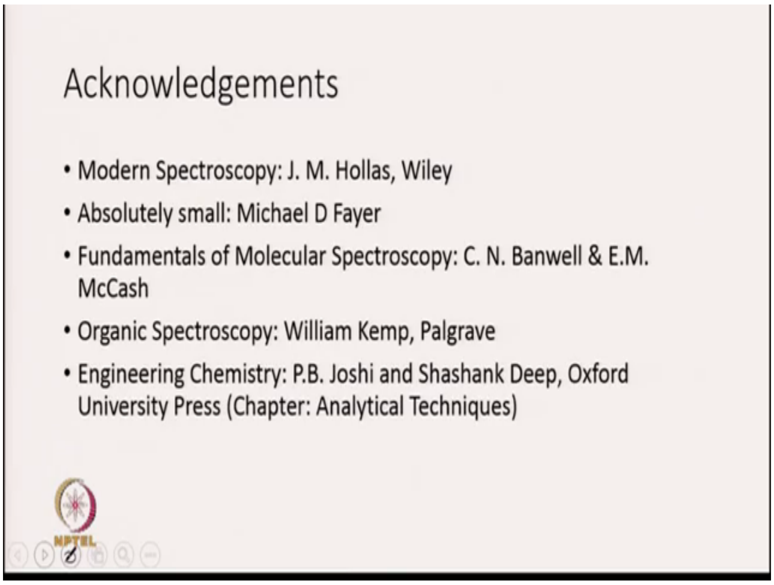

So since now time is over so I will not be discussing hermitian operator I will discuss in the next class so thank you for listening thank you for listening and go to last slide I like to acknowledge these books which I am referring to and thank you very much for listening see you in the next lecture thank you.