Quantum Mechanics - I
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Lecture - 27
The Particle in a one-dimensional Box

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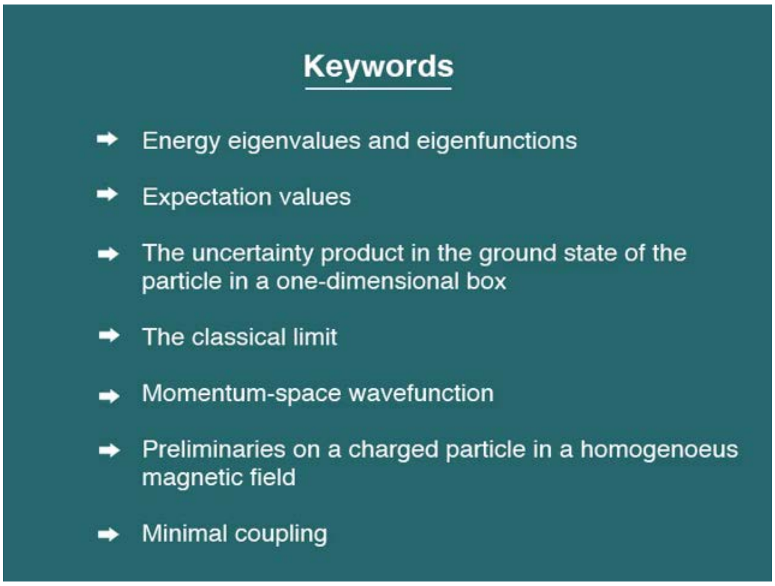

In my last lecture, I spoke about the one dimensional potential barrier. Of course, earlier on we had discussed the one dimensional square well potential. Now, in the potential barrier problem, towards the end, we realized, that the probability of tunneling went down exponentially; If the value v 0, the value of the potential, the magnitude of the potential, was much larger than the energy of the particle, which is trapped on one side of the barrier. Question asked is, what is the penetration across the barrier? And, this would exponentially come down if the energy of the particle is significantly smaller than v naught.

In other words, as the height of the barrier increases the probability of tunneling, the probability of leakage across the barrier goes down and goes down exponentially. So, we will remember this and do yet another example, of stationary state, a one dimensional problem, where this time we will discuss, a particle in a box. It is a much simpler example, than all that we considered earlier, in the following sense, that we imagine this particle of mass m to be inside a box. The walls of the box are impenetrable. So, basically you have infinite barriers, for the walls of the box. But, the operator word is this; within the box the particle is free to move anywhere. It has positive energy e. The total Hamiltonian is p square by 2 m, where p is a linear momentum of the particle, but then there is no barrier penetration.

The walls of the box behave like, infinitely high barriers and therefore, in the region outside the box, you will not be able to see the particle.

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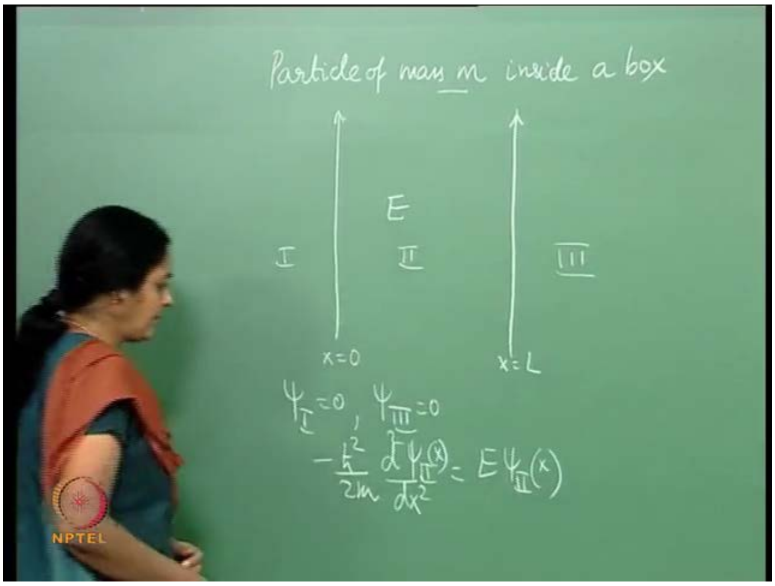

And therefore, in the case of the particle in the box, suppose, I have these infinite barriers, at x equals 0 and x equals L. The particle is confined between these two regions, these two barriers and I call these regions: 1, 2 and 3. This is a particle of mass m inside a box, psi 1 is 0, psi 3 is 0. Inside here there is no potential. The particle has energy E, it is a free particle and therefore, in region 2, I have an equation minus h cross square by 2 m, d 2 psi 2 of x by d x square, is e psi 2 of x.

What are the boundary conditions that we can impose? Certainly, the wave function must be continuous. So, at x equals 0 and x equals L, we will impose continuity of the wave function. But then, because of this infinite barrier, here there are infinite discontinuities here and there and therefore, you cannot expect the 1st derivative of the wave function to be continuous. That will show a finite discontinuity. So, we shall not impose the derivative matching condition at x equals 0 and x equals L. We will merely work with the fact that the wave functions will match; psi 1 equal's psi 2 at x equal's 0 and psi 2 equal's psi 3 at x equal's L.

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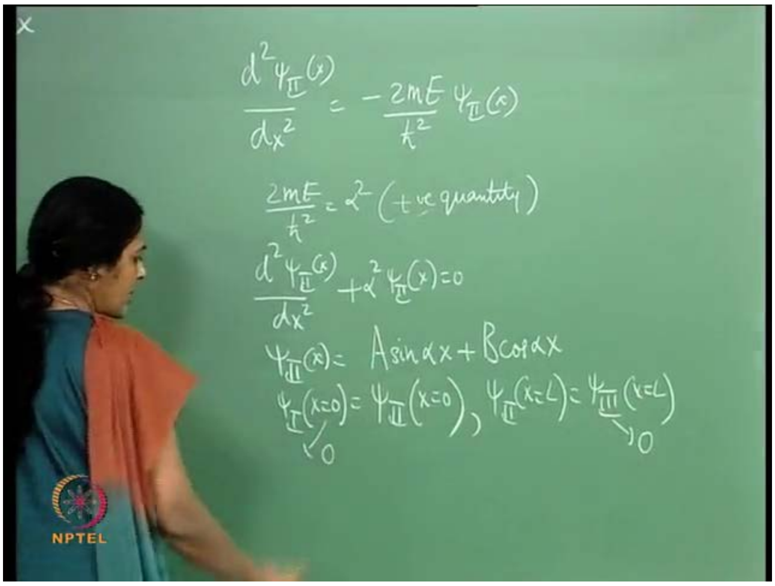

So, looking at psi 2, we have d 2 psi 2 of x, by d x squared, equals minus 2 m E by h cross squared, psi 2 of x and, let us call 2 m E by h cross squared. As alpha squared, which is a positive quantity; and therefore, I have d 2 psi 2 of x, by d x squared, plus alpha square psi 2 of x equals 0. Which, leaves me with a plane wave solution inside the box, because, it is a free particle. I could well write this, as psi 2 of x is A sin k x, alpha x plus B cos alpha x, psi 1 is 0 and psi 3 is 0. When I say psi 2, this is the wave function within the box (Refer Slide Time: 02:24) that is between x equals 0 and x equals L.

So now, let us match the wave functions at the boundaries, psi 1 at x equals 0 equals psi 2 at x equals to 0. I have selected the box, to range between 0 and L and psi 2, at x equals L equals psi 3 at x equals L. But, this quantity is 0 and this quantity 0. I therefore, have the following boundary conditions which will simplify my wave function.

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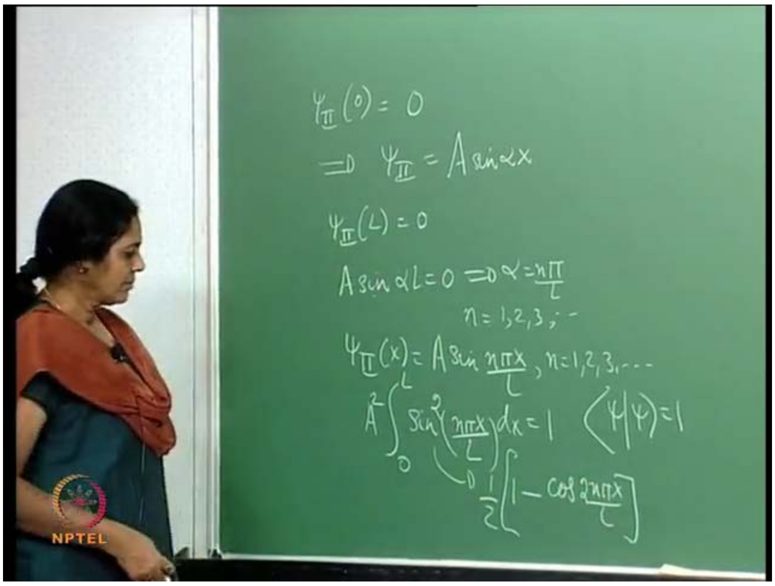

So, psi 2 of 0 out there, when I match it with psi 1. This simply implies, that the cos function out here, (Refer Slide Time: 04:30) B cos alpha x, does not contribute at all. Because, cos 0 is 1 and therefore, B must automatically be 0 and that tells me, that psi 2 is A sin alpha x.

Of course, A is the normalization; we will have to determine that. At x equal's L, I have psi 2 of L equals 0, because psi 3 is 0. That tells me, that A sin alpha L equals 0. Since, A in general is not 0, because, then the wave function itself will vanish. I have alpha equals n pi by L, where n can take values, I cannot put 0, because, if n were 0 then alpha is 0. Recall that the energy (Refer Slide Time: 04:30) is related to alpha. Alpha square is 2 m e by h cross squared and then the energy will be 0.

So, n is equal to 0 is not an allowed solution. On the other hand, n equals: 1, 2, 3 also plus minus, plus minus 1, plus minus 2, plus minus 3 in general. But, if n is minus out here, it simply going to give me the same function, because sin of minus x is minus sin of x. I do not get anything independent. That is just an overall phase that will come out and therefore, this is the solution. Alpha is n pi by L, where n takes values: 1, 2, 3 and therefore, psi 2 of x, is A sin n pi x by L.

I have to determine A, the normalization constant. The normalization is done by looking at the entire interval. But, from minus infinity to 0, psi is 0. So, that does not contribute. Again from L to plus infinity the wave function vanishes. So, there is no contribution.

The only non 0 contribution I need to worry about, is integral 0 to L, A squared psi star of x psi of x, which is psi sin squared n pi x by L d x. This quantity is normalized to 1. This is in fitting with the probabilistic interpretation. Because, this is a same as saying, that this object is equal to 1. Let us recall, that because we are working in the position representation, I have integral psi star of x psi of x d x equals 1. And, that should determine A square for me. Because, I could of course, write this as half 1 minus cos 2 n pi x by L and do the integration.

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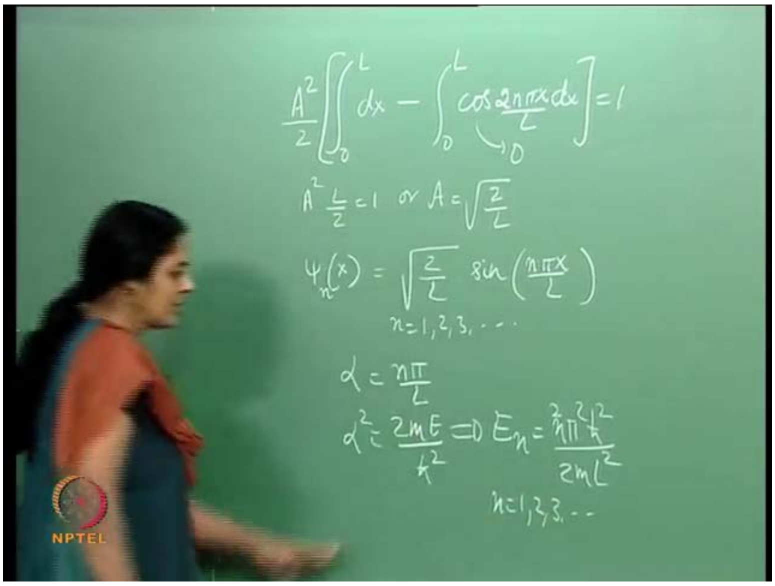

So, that tells me, that a square by 2 integral d x from 0 to L, minus integral cos 2 n pi x by L d x. This quantity is 1. That is not going to make a contribution and this gives me just an L. So, A squared times L by 2 is equal to 1, or A is root of 2 by L. I have not chosen minus root of 2 by L, because wave functions anyway are arbitrary up to a phase. And therefore, my wave function, I will drop this suffix, this subscript 2 out here and I will write psi of x is root of 2 by L sin n pi x by L, n is 1, 2, 3 and so on.

So, this is a wave function psi of x, I should in fact put psi n of x out there, Because, there are very many states, Eigen states of the Hamiltonian, because this is indeed the solution to the Schrodinger equation. What are the corresponding energy levels? We decided that alpha was n pi by L and since alpha squared is 2 m e by h cross squared, which implies that E sub n, is n squared pi squared h cross squared, by 2 m L squared, n taking values 1, 2, 3 and so on. So, these are the Eigen functions. So, if you put a particle in the box, there are discrete energy levels. Call them E sub n and the expression is e n is n squared pi square h cross square by 2 m L squared. And, the corresponding wave functions, are given by root of 2 by L sin n pi x by L. So, that is what we have.

Now given this, we would like to see what the uncertainty product is like, specifically in the ground state of the particle in the box, because, we know that for the harmonic oscillator problem, the one dimensional oscillator problem that we have already handled. The ground state was a minimum energy state, minimum uncertainty state and delta x was equal to delta p. And, the uncertainty product got equalized in the ground state. So, let us see what happens here. So, the aim is to calculate, the uncertainty product, in any state of the particle in the box.

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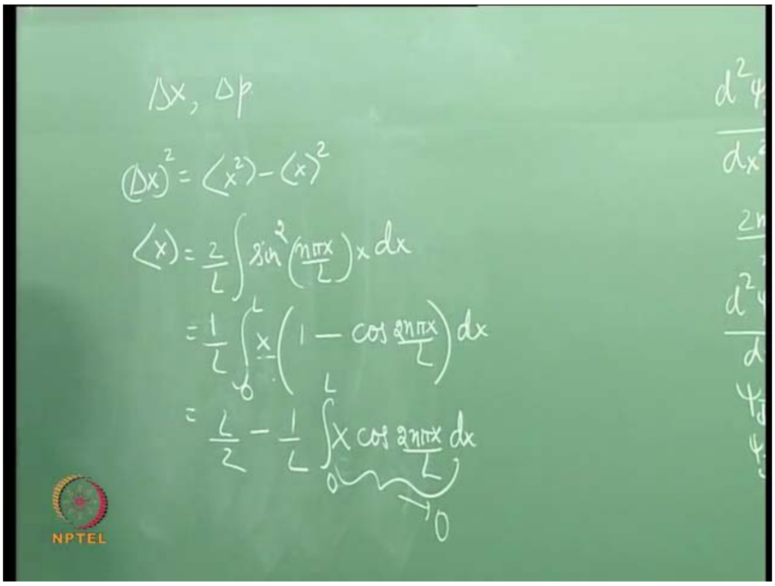

So, we need to compute delta x and delta p. Recall that delta x squared, is expectation x squared minus expectation x, the whole square. Similarly, delta p squared. So, we begin with expectation x. The expectation value of x in any state is integral psi star x psi. So, that gives me a 2 by L, sin squared n pi x by L times x d x.

Now, before I compute this integral, I would like to argue and find out, what would be the value of x? So, this particle is not biased towards any particular point or in any particular direction. It is a free particle moving anywhere within the box and incapable of penetrating outside the box. In that case, on an average you would expect that x would take the value L by 2, because, that is the average of 0 and L. So, I would expect the mean value of x, to be L by 2. We can always do this calculation explicitly and see if indeed that is true. This is 2 by L, integral x 1 minus cos 2 n pi x by L, d x by 2. And therefore, I might as well write this as 1 by L times this, where the 1st term in the integral from 0 to L is just, integral x d x and this is from 0 to L.

So, the 1st term just gives me an L by 2, which is what I thought, would happen. But, I have another integral, which is minus 1 by L, integral x cos 2 n pi x by L d x. You can use integration by parts and that quantity vanishes. It is a trivial integration and indeed my guess was right that expectation value of x is L by 2. So, an average the particle has no preferred direction, moves anywhere inside the box. Like a free particle, not subject to any potential and therefore, the average value of x, would be L by 2. Because, the boundaries, where at x is equal to 0 and x equals L.

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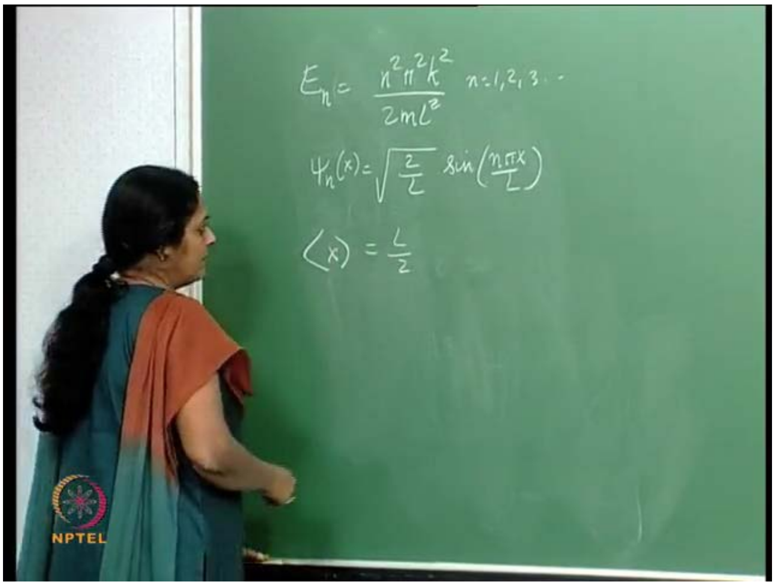

So, let us put that down somewhere, we have E n is n squared pi squared h cross squared by 2 m L squared, n equals, 1 2 3 and so on. And, psi n of x, is root of 2 by L, sin n pi x by L. Expectation value of x in the state psi sub n, is L by 2. So, it seems to be independent of which excited state the particle is in. That is all that we have. But, expectation x squared is not so trivial. We can compute the integral and that is going to be a function of n. And therefore, there is going to be a variance, which gets a contribution both from the mean value of x and from x square’s expectation value. So, let us compute that.

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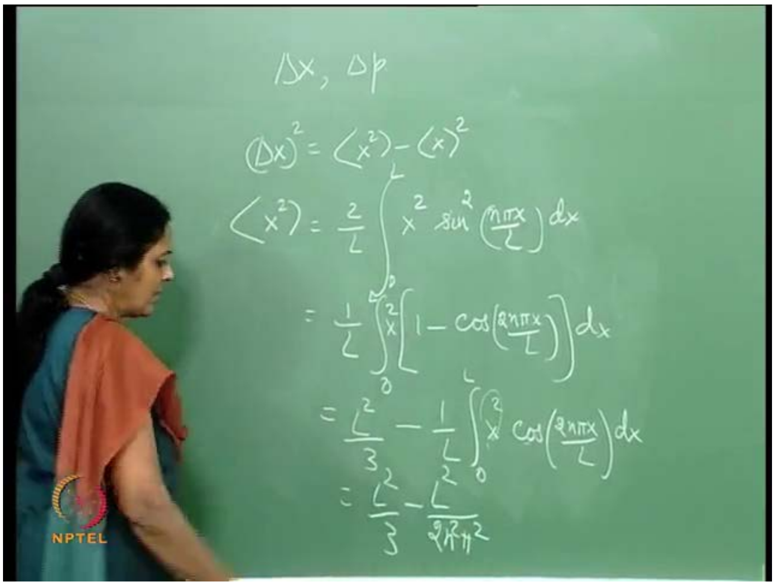

Expectation x squared is of course, 2 by L, integral x squared sin square n pi x by L d x. This object is again 1 by L, integral 1 minus cos 2 n pi x by L, x square d x. The integral of course, goes from 0 to L. Well, the 1st term, gives me an integral x squared d x, which just gives me an L squared, by 3 with the 1 by L. Then I have a minus 1 by L integral 0 to L x squared, cos 2 n pi x by L d x. This integral again can be worked out explicitly. You can use integration by parts, call this u, call that d v.

So, if that is d v, cos 2 n pi x by L d x, if that is d v, v is a sin. So, the term u v has x squared sin 2 n pi x by L and then there is an integral v d u, which will make a contribution. And you can simplify this, it is a simple integral and the answer is minus L squared by 2 n squared pi square being the contribution from here. So, this is what we have for expectation x square. As you can see, there is an n dependence, in the expectation value of x squared. And, for large quantum numbers, the contribution from this term goes down. This is a point I will comment on a little bit later. So, let us put down that result.

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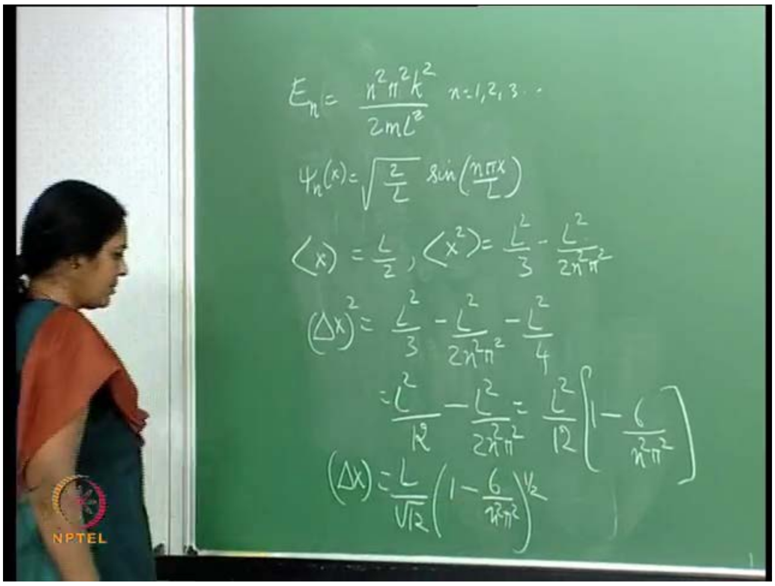

This is L squared by 3 minus L squared by 2 n square pi square, where of course, one should be careful with dimensions. If you are talking of expectation x, it has to be the 1st power of L. If it is expectation x squared, the dimension comes from L squared. And therefore, delta x the whole squared is L square by 3 minus L squared by 2 n square pi square, minus L square by 4, from expectation x the whole squared, which is L square by 12, minus L square by 2 n squared pi squared. This is what I have and therefore the variance. So, I can well write this as L square by 12 times 1 minus 6, by n square pi squared. That is the variance and therefore, delta x is L by root 12, 1 minus 6 by n square pi squared, to the power of half. So, that is what I have for delta x.

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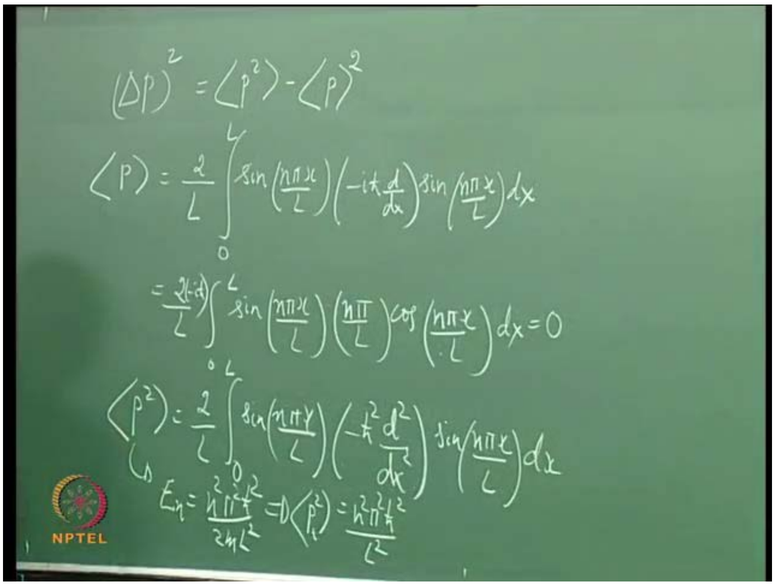

So now, let us find the variance in p. So, delta p the whole squared that is the square of the variance, as you know is expectation p squared, minus expectation p the whole square. So, what is expectation p? This object, my wave function is root of 2 by L sin n pi x by L. So, I pull out a 2 by L, integral sin n pi x by L. I write p in the position representation, as minus i h cross d by d x. So, that is a psi star psi, of course, the integral limits go from 0 to L.

The wave function is a real wave function and therefore, psi star is the same as psi and we are working in the position representation. So, this object apart from a minus i h cross, which I can pull outside, is simply sin n pi x by L, n pi by L cos n pi x by L d x. And this integration, if I do it, I will get 0. In fact, I can come up with a very reasonable argument, as to why this should be 0. Because, the particle will caught in a square well, will move as much to the left, as to the right and so on an average, I would expect the net momentum to be 0.

On the other hand, there is a contribution from expectation p squared, to the square of the variance. So, once again I can find this, as before, I have psi star psi. But, now it is a minus h cross squared d 2 by d x squared, sin n pi x by L. Because, I have substituted for p squared, I could do this integration. On the other hand, I can come up, with a nice argument, as to what it should be. Look at expectation p squared. Now, E sub n is n squared pi squared h cross squared, by 2 m L squared. And therefore, p squared you know that E is p squared by 2 m and therefore, p squared is m squared pi squared h cross squared by L squared. In fact it is p n and this is what makes a contribution, to delta p squared. Not from here, but from expectation p square. Of course, I can explicitly work out this integral and if I did, that I would get this answer.

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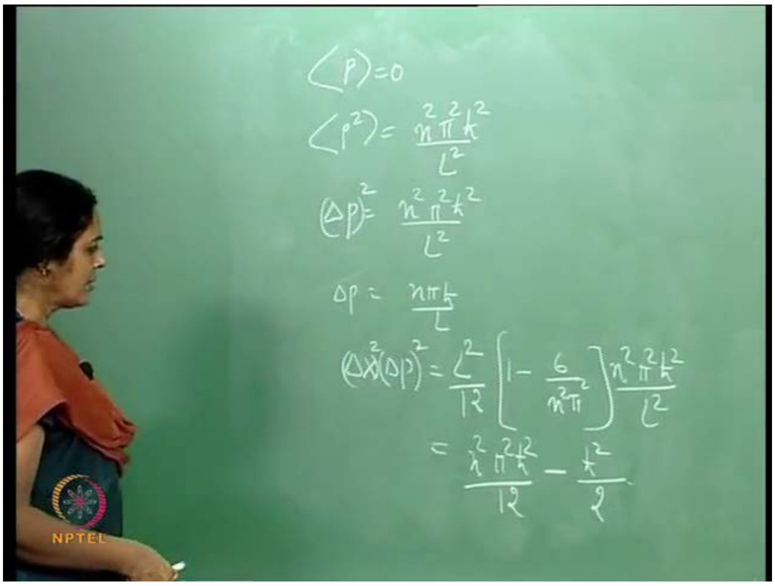

So, let us write that down here and expectation p squared, is n square pi square h cross squared, by L squared. I can now compute delta x. Delta x is simply expectation p squared, delta p. That is simply expectation p squared and that is n squared pi squared, delta p the whole squared, is n squared pi square h cross squared by L squared. And therefore, delta p is n pi h cross by L. I now compute the uncertainty product delta x delta p in the state psi n. I have got delta x there. (Refer Slide Time: 16:06) So, it is easier to do delta x squared delta p squared.

So, delta x squared is out here. It is L squared by 12, times 1 minus 6 by n squared pi squared, times delta p square which is n square pi square h cross squared by L squared. And, that gives me quantities, the 1st one depends on n square and if the 2nd one you will see that n square cancels out. The 1st one, the L square cancels out and I get an n squared pi squared h cross square by 12, minus h cross squared by 2. We can therefore, now find, the value of the uncertainty product, say in the ground state of the particle in the box, setting n equals 1.

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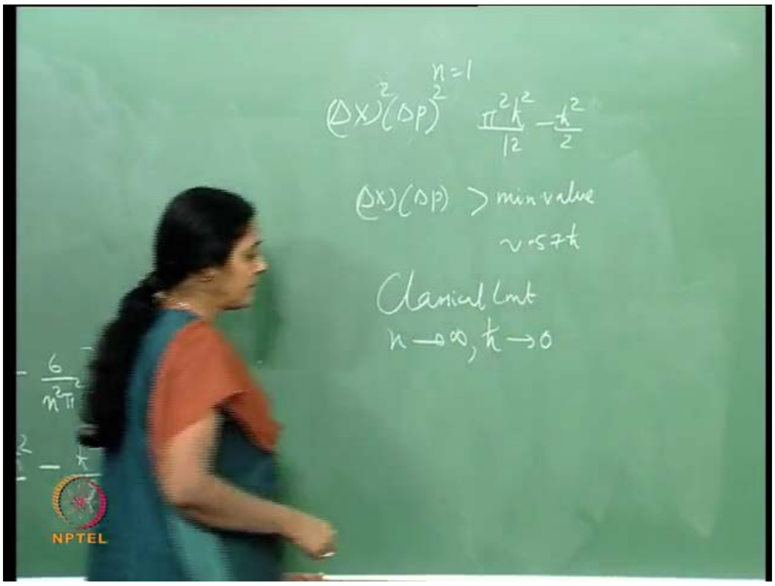

So, let us do that, delta x, delta p, in the ground state for n equals 1. So, (Refer Slide Time: 24:33) delta x squared delta p squared, is pi squared h cross squared by 12, minus h cross squared by 2. We can now put in the value of pi and you can see that the uncertainty product delta x delta p, is greater than the minimum value, because it is roughly 0.57 h cross. This is there for not a minimum uncertainty state.

It is obvious that the higher energy states are even worse and there is no minimum uncertainty state, in the case of the particle in a box. The ground state is not a minimum uncertainty state and the other states are even worse. (Refer Slide Time: 24:33) In the sense delta x delta p is larger than, its value for the ground state. You can substitute n is equal to: 2, 3, 4 and so on out here. There is an interesting observation that one can make at this point.

How do you go to the classical limit of the problem? In classical mechanics, the energy levels are not discrete, they are not quantized. Now, for this particle in a box, the energy level must be a continuum of numbers and when do I hit the classical limit. I hit the classical limit, of course, (Refer Slide Time: 24:33) when n becomes very large, h cross has to go to 0 to get to the classical limit. So, the classical limit is reached, for n going to infinity and h cross going to 0.

At that stage, I would really retrieve the classical features. Because, the difference, (Refer Slide Time: 24:33) between n plus 1 the whole squared and n squared, goes down.

For large n, compared to values where n is small and therefore, as you consider larger and larger values of n. It is clear, that the energy levels get closer and closer to each other. This is simply a constant.

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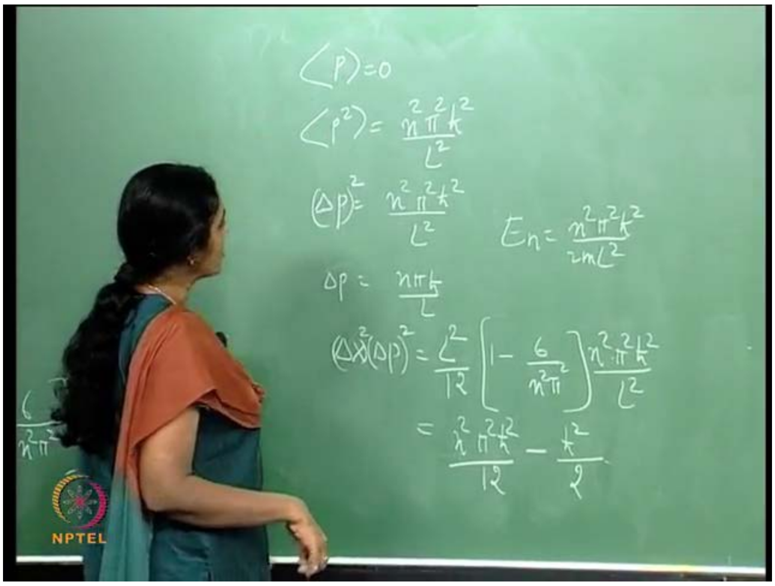

The energy levels get closer and closer to each other, if you look at E sub n and you no longer see the separation very clearly. In other words, you hit the continuum, or you have, hit something that looks like a continuous stretch of states, or you have hit the classical limit.

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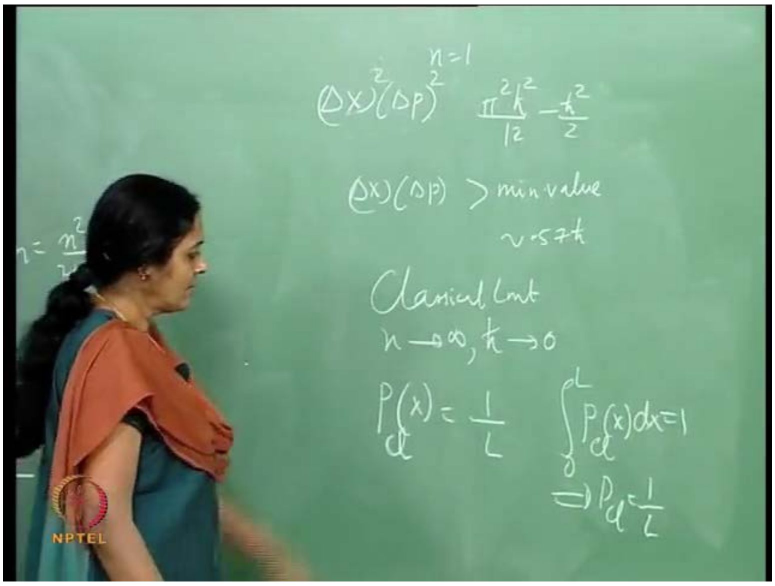

So, now let us look at the classical limit of this problem. What exactly happens in classical physics? In classical physics, I can talk of the probability distribution, of x and so on. So, let us look at the probability distribution. The probability distribution of x, would be uniform, in classical physics for this problem. Because, the particle can be anywhere, with equal probability and therefore, p of x, let me call it p classical of x.

This would be 1 by L, anybody is guess, because you know that the total probability has to be 1 and that of course implies, that p classical, is 1 by L. That gives me an integral d x which is an L and things neatly cancel out. So, if this is p classical, I can find out the value of the mean value of x, the mean value of x squared and so on, in classical physics.

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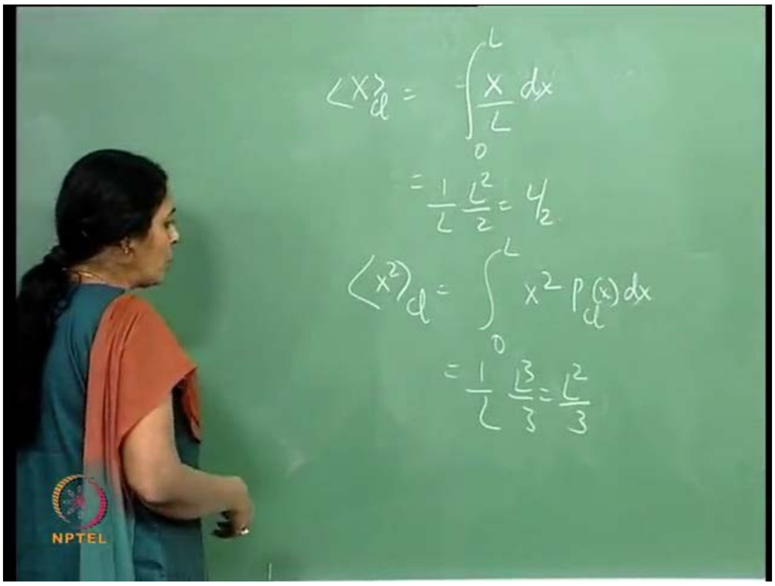

So, the mean value of x, let me call that x classical, the mean value x classical. This object is simply integral x p classical, d x from 0 to L and that is 1 by L, L squared by 2, which is L by 2. So, both in classical physics and in quantum physics, I would expect this to be the average value of the position, L by 2. Not surprisingly therefore, even in the classical limit, the quantum value is simply the same as the classical value. It is L by 2. Now, look at expectation x squared classical, I use this notation to show the average value in classical physics.

Now, that is 0 to L x squared p classical of x d x. That is 1 by L, x cube by 3, between 0 and L. So, that is L cube by 3, which is L square by 3. This is what I have, for expectation x squared classical, that is L squared by 3. Now, look at the expectation value of x square here. (Refer Slide Time: 19:10) In the quantum mechanical analogue, where the particle was a quantum particle in the box, you have an L squared by 3, minus L squared by 2 n squared pi squared. Now, in the limit of large quantum numbers, for n going to infinity, you find that expectation x squared quantum goes to the classical limit, which is given here, which is L squared by 3. So, that is one thing that we have checked out.

Now, look at expectation value of p, I would use the same argument that I used in the quantum case for expectation value of p. The particle can go anywhere, to the right and to the left, with equal probability and therefore, on an average I would expect it is momentum to be 0. The velocities to the right and to the left would be occurring with equal probabilities. And therefore, I would expect the expectation value of p to be 0, as to delta p itself, in the quantum case.

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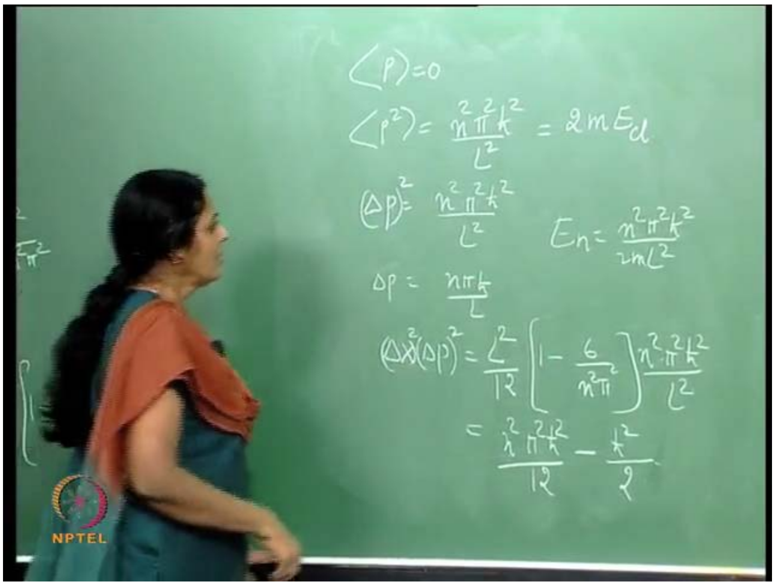

I have delta p to be essentially given by expectation p squared, because expectation p was 0 and expectation p squared, is delta p the whole squared, which is n squared pi squared h cross squared, by L squared and what should it be? I know that, this should simply be 2 m E classical. Because, p squared by 2 m is indeed E classical, in the classical case. And therefore, expectation value of p squared square root gives me delta p, which should be square root of 2 m E classical.

So, this is the way one goes, from the quantum case to the classical limit. There is one very interesting aspect, so much for the uncertainty. There is one very interesting aspect to this problem and that comes by looking at the momentum space, wave function and the probability density in momentum space. The momentum space wave function, is clearly obtained by doing the Fourier transform of the position space wave function.

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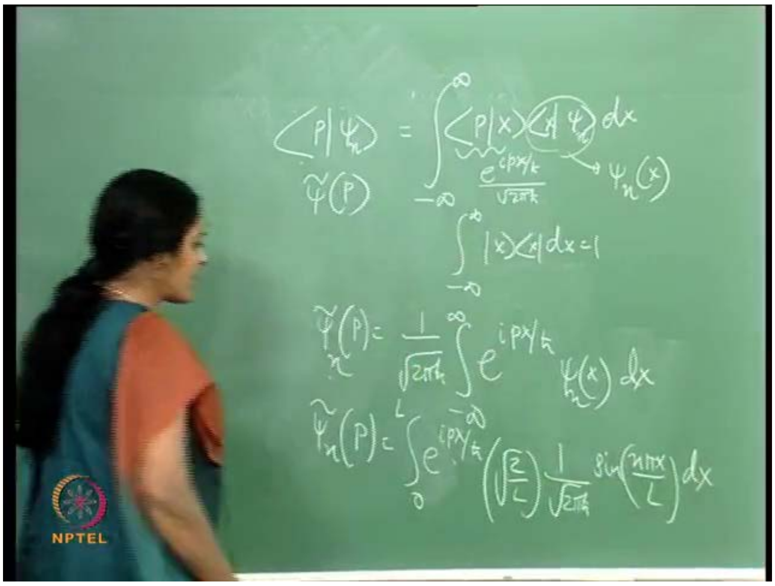

So, in the Dirac notation for instance, I would denote the momentum space wave function, psi tilde of p, as this inner product, bra p with ket psi. This can well be written as p x x psi, I am talking about quantized energy levels and therefore, I might as well write psi n d x. Really this should go from minus infinity to infinity, in general and I have introduced a complete set of states. The right hand side is the identity operator. This object, here is simply psi n of x. It is the n-th Eigen state, in the position representation. But, I know that psi tilde of p is related to psi n of x through the Fourier transform.

So, basically this object here, is e to the i p x by h cross. But, I would also do a root of 2 pi h cross. That is when I go from the position space to the momentum space. I have psi tilde of p, is equal to 1 by root of 2 pi h cross, integral over the allowed values of x, e to the i p x by h cross psi of x. I should really write psi n tilde of p, if I have psi n of x d x. The root 2 pi here is of course a convention, because, I could have put a 1 by root 2 pi h cross here and when I do the inverse Fourier transform, I would put a 1 by root of 2 pi h cross, when I go from psi tilde the of p to psi of x.

I could instead not have the 1 by root 2 pi at all in one case. I could have made this 2 pi h cross and nothing out there, just one out there, when I go from the momentum space to the position space. Equally, I could have kept 1 here as a coefficient removed this and I could have transferred 2 pi to the other side and so, when I come from the momentum space to the position space during an inverse Fourier transform. I could introduce a coefficient 1 by 2 pi. So, those are conventions, now, use this convention and this is what I have.

So, this is the momentum space wave function, except that now, I need to put in psi n of x. Between, excess 0 and excess L and therefore, psi n tilde of p is really going to be integral 0 to L, e to the i p x by h cross, root of 2 by L, 1 by root of 2 pi h cross, sin n pi x pi L d x. So, this is the integral that one has to do, in order to find psi n tilde of p, the momentum space wave function. One can do this integral and find modulus of psi n tilde of p the whole square and that is going to be the momentum space, probability density.

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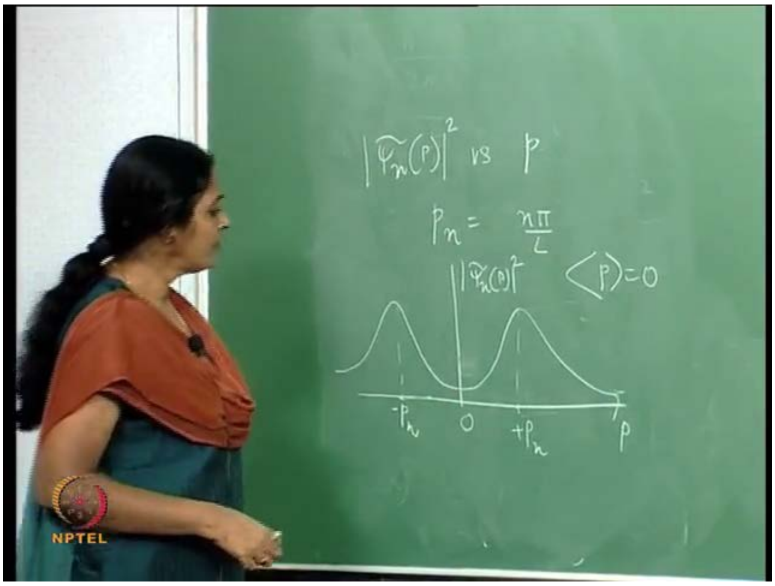

So, if you plot that distribution versus p, you see something pretty interesting. Modulus of psi n tilde of p, the whole squared can be computed and if you plot modulus of psi n tilde the of p, versus p. Defining p sub n as n pi by L, the plot of modulus of psi n tilde of p, the whole squared versus p, takes a maximum asymmetric first of all. It takes a maximum, at plus p n and minus p n. At these two values, plus p n and minus p n, mod psi n tilde of p the whole squared, picks up maxima and interestingly the minimum value is at p equal to 0.

This is a point to note, because expectation value of p was 0. While the mean value of p 0, p 0 is the lowest probability point. Because, you find that the probability distribution really peaks up at p is plus n, plus p n and minus p n. So, the average value is really the lowest probability value. For this distribution and that is a very important and interesting point to remember in the context of the case of the particle in the box. So, we have seen three situations. The particle in the box, the square well potential and the infinite potential barrier. These are all examples of stationary states and several interesting quantum properties emerged in the process.

There was tunneling, leakage across the well, into the classically forbidden region, tunneling across the barrier. The manner in which the quantum limit went to the classical limit, the classical limit itself comes for large quantum numbers, where n goes to infinity and h cross goes to 0. We have seen the free particle solution, psi is a plane wave solution e to the i p x by h cross, or e to the minus i p x by h cross. We have seen the harmonic oscillator, the 1 dimensional oscillator where we had the ladder operators b and b dagger and we had discrete energy levels and essentially the Hermite polynomials, as the energy Eigen state. Now, to a last and very interesting problem in this category and that is the case of a charged particle, in a homogenous magnetic field.

You will find that this spectrum, in a sense, has a part which behaves, like the linear harmonic oscillator spectrum and another part, which behaves like the free particle. So, there is a combination of both the harmonic oscillator and the free particle, in the case of the problem of the charged particle of mass m, moving in a homogenous magnetic field. So, let me just set up the foundation for that and then in tomorrow’s lecture, I can look at the details of this problem.

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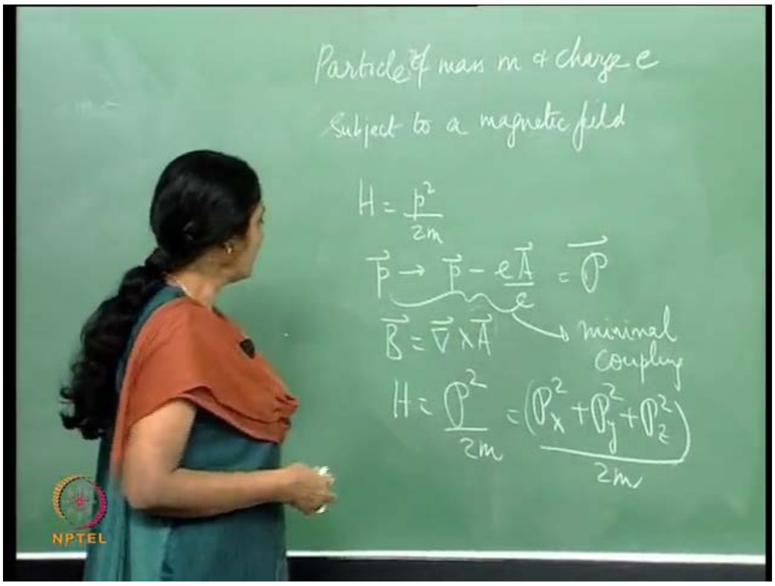

So, we now discuss the problem of a charged particle, in a homogenous magnetic field. Particle of charge, particle of mass m and charge e, subject to a homogenous magnetic field, subject to a magnetic field, where we will approximate, we will simplify it to a homogenous magnetic field, a little later.

The Hamiltonian for a free particle is p squared by 2 m, as you know p is a linear momentum of the particle. Now, in the presence of a magnetic field, you do a minimal coupling and p itself, is replaced by p minus e A by c, where A is the vector potential. The magnetic field itself is related to A, by B equals del cross A. So, let me call this as P not pi, P like that. The Hamiltonian then, is P squared by 2 m, where P is defined. The vector P is simply the linear momentum of the particle, minus e A by c. This prescription p goes to p minus e A by c. Leads to something called the minimal coupling, because, when you do the squared. There are terms, which involve p dot A, A dot p and so on. And, that is the coupling, between the particle that momentum p and the vector potential A, of the field.

That we are talking about and, this is a minimal coupling, one can think of more non minimal terms, but that is beside the issue right now, we shall work with the minimal coupling prescription. So, this is obviously going to have 3 components, P x square plus P y square, plus P z squared, by 2 m. Now, it is clear, that the magnetic field is the physically observable field. Is a physically observable quantity and not so much the vector potential A, in the sense, that several A’s, in fact, an infinite set of vector potentials could give me the same magnetic field. Because, if I replace A, by A plus gradient of a scalar quantity, I would still get the same B.

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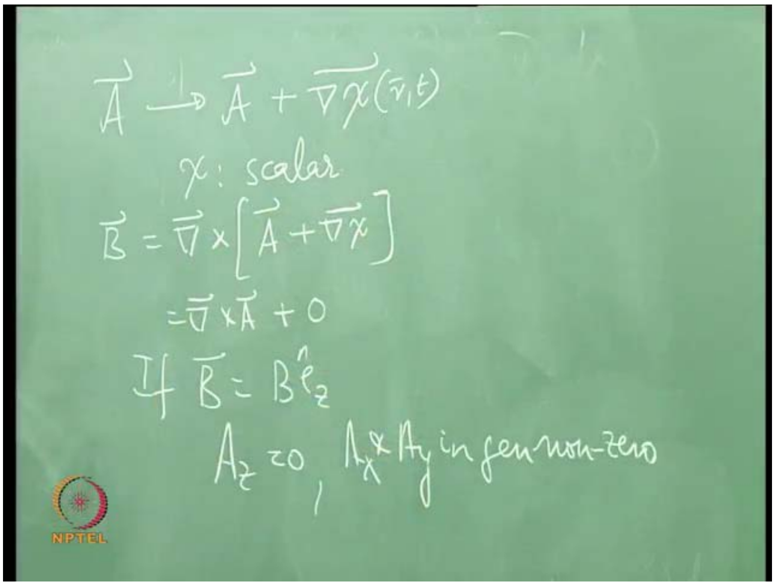

So, I can do what is called, a Gauge transformation, on A. A goes to A plus grad chi, chi is a function of space time and chi is a scalar. Then B is now del cross A plus grad chi, which is del cross A, plus the curl of a gradient and that is 0. And therefore, there are in principle, I can choose chi to be anything I wish, any scalar function and therefore, for an infinite set of vector potentials, I get the same magnetic field B.

The Hamiltonian (Refer Slide Time: 42:01) is given in this manner. I would like to make this magnetic field homogenous. In the sense, I would like to choose B to be, a constant magnetic field, independent of space and time, along the z direction. The direction of B is chosen as a reference axis, or the z direction. Now, in that case, A z will be 0, because, b is equal to if B is equal to B e z, A z is 0 and A x and A y in general non zero. It is possible for me, since, I have already explained that different A’s could lead to the same B. It is possible for me to choose A x and A y non zero, for a given B. I could choose A x to be 0 and A y to be non zero, for the same B, or A x to be non zero and A y to be 0, get the same B.

So, by Gauge transformation that is by changing a given value of A, to A plus grad chi and choosing my chi appropriately. I can have a different an infinite set of vector potentials, which will give me the same B. I choose a Gauge, by fixing a certain value, of A x, A y and A z. In this case A z is 0 and depending upon the choice of A x and A y, I would say that I have selected a Gauge. So, we will work out the problem of the particle in the homogenous magnetic field. Get the Eigen spectrum, the energy Eigen spectrum and the Eigen values, for specific Gauges, that means for specific choice, of A x, A y and of course, A z is equal to 0. This is what we will see in the next lecture.