Path Integral Methods in Physics & Finance

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Lecture – 23
Equivalence of Schrodinger & Path Integral Formalisms, Matrix Elements of Operators

Welcome back. In the last lecture, we obtained certain very interesting results; we obtained the expression for the propagator of the harmonic oscillator and the free particle using the path integral approach. Before we proceed further, it would be opportune at this point to discuss the equivalence of the Schrodinger Formalism and the Path Integral Formalism.

So, let us start with that today and then, we will proceed to work out the time ordered products and the expectation value for the time ordered products in the path integral framework.

So, that is the agenda that I have for today; time permitting, I will also discuss a little bit more about the features the properties, the nuances of the path integral. But let us start with the equivalence between the Schrodinger and the path integral framework.

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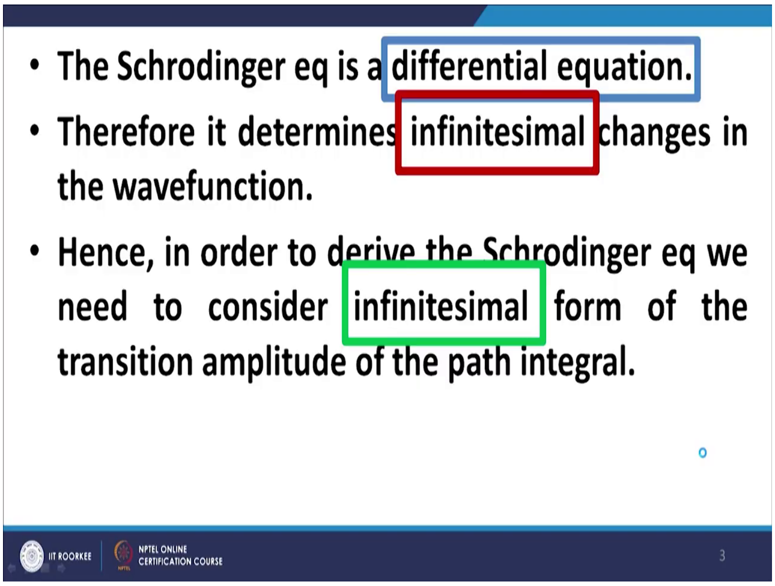

Now, the first thing is that the Schrodinger equation is a differential equation. So, being a differential equation, it relates to time evolution or it provides an expression for the time evolution at the infinitesimal level. In other words, it gives you the infinitesimal evolution in terms of time and in terms of the wave function. So, that is what we have to keep at the back of our mind, when we try to establish the equivalence. The Schrodinger equation is a differential equation and therefore, we have to deal with infinitesimals.

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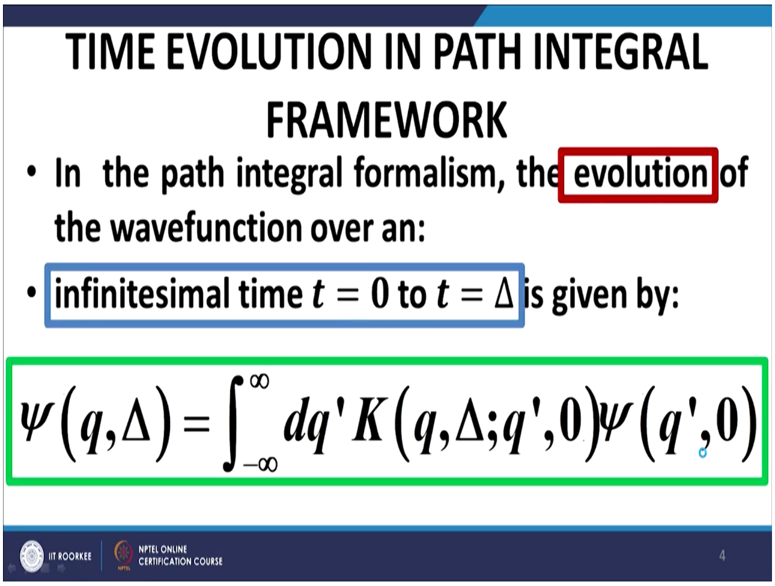

Now, as far as the path integral framework is concerned, the expression for the evolution of a state from t equal to 0 to a small t equal to delta is given by the expression in the green box. There were this K q delta q delta is the transition amplitude and this expression gives you the time evolution in the path integral framework.

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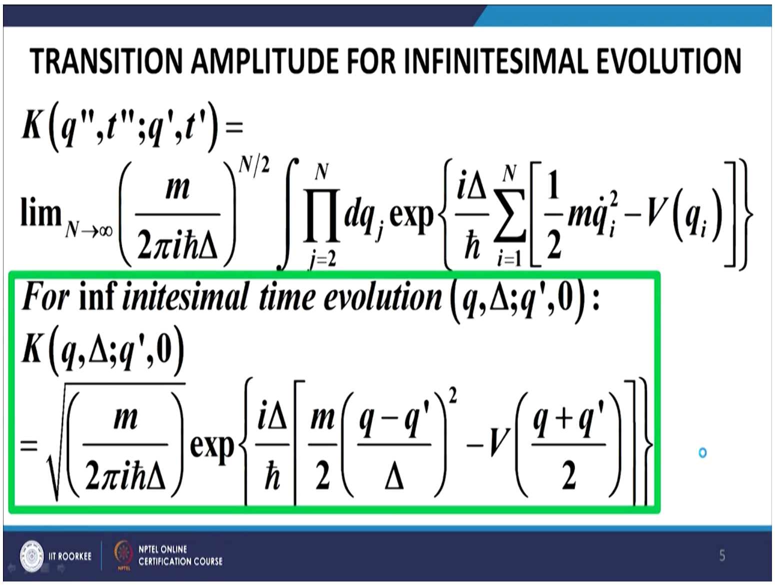

ah Now, for the transition amplitude and the expression that we have derived for the transition amplitude in the path integral framework is the first equation given on your slide. This is what we obtained in the previous lectures for the Feynman's path integral in configuration space. For infinitesimal time evolution, obviously, this equation simplifies a bit and we have to retain only the portion that is there in the green box. For i, reiterate the fact that the expression in the green box holds for infinitesimal for very small time evolution, where the evolution time is very very small.

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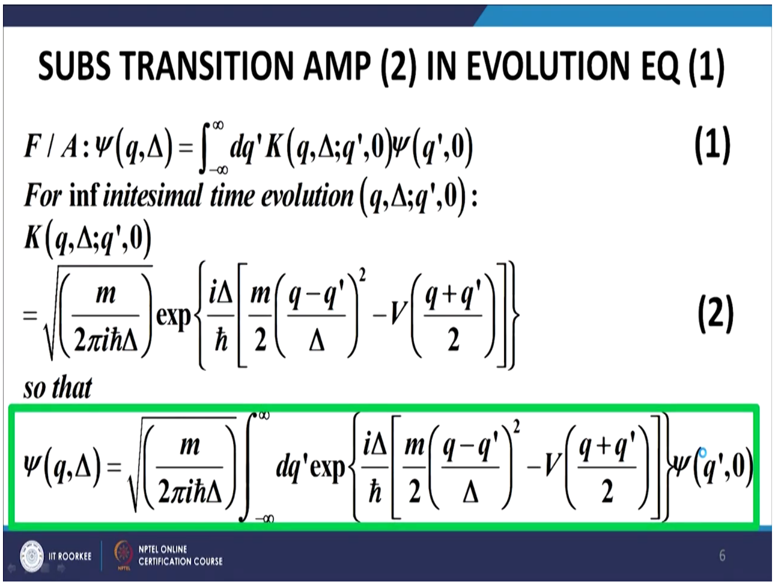

Now, substituting the transition amplitude 2 that is the what we had in the previous slide, this green box expression. This is expression 2. In the expression 1 which we have originally for the time evolution in the path integral framework, we get the expression which is here in the green box right at the bottom of your slide and so, this is what ultimately, we have to manipulate and we have to put it in a form which is compatible or which is equivalent to the Schrodinger equation.

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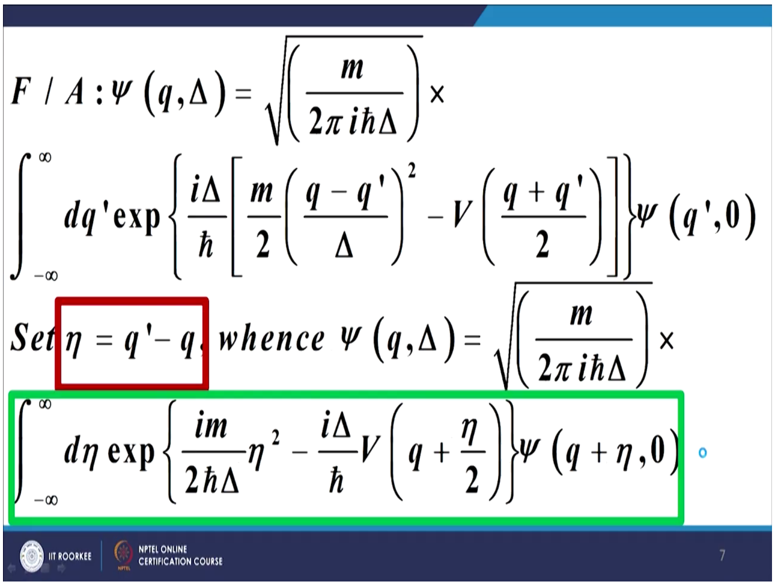

So, this is what we have. This is what we have from the previous slide. We to introduce compatibility of notation or convenience of notation rather we introduce eta as the expression q dash minus q. And in terms of eta we write down obviously the integration element changes from d q dash to d eta, q being stationary and we get the expression which is there in the green box on making this substitution.

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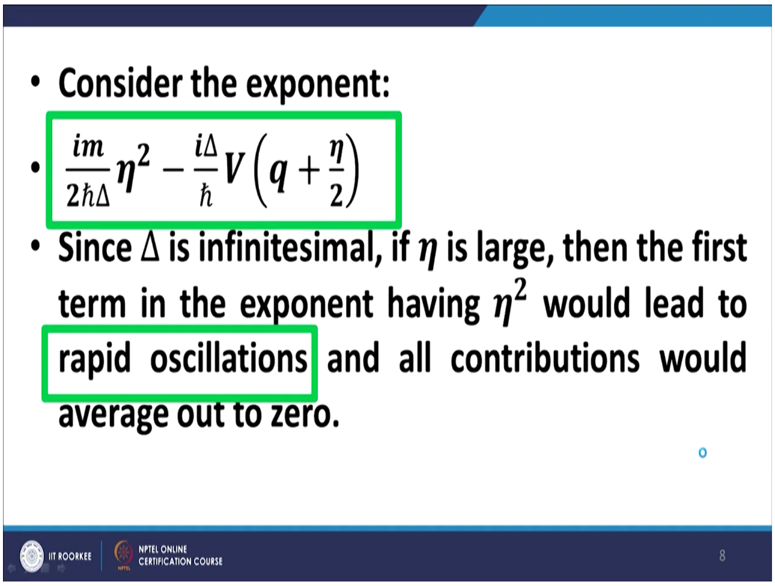

Now, let us consider the this exponent, the exponent of the exponential as exponent e to the power the curly brackets im upon 2 h delta eta square minus i delta h V q plus eta by 2. Let us look at this expression, let us look at the behavior, the qualitative behavior of this expression.

Clearly, since delta is infinitesimally small, large values of eta would result in the this integral, this whole expression, this exponential being are showing rapid oscillations. And as a result of which rapid, as a result of these rapid oscillations what will happen is that the contributions, overall contributions will be nearing zero.

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- The dominant contribution will, therefore, come from the the following region where the change in the first exponent is of order of unity:

$$\boxed{0 \le |\eta| \le \left(\frac{2\pi\hbar\Delta}{m}\right)^{\frac{1}{2}}}$$

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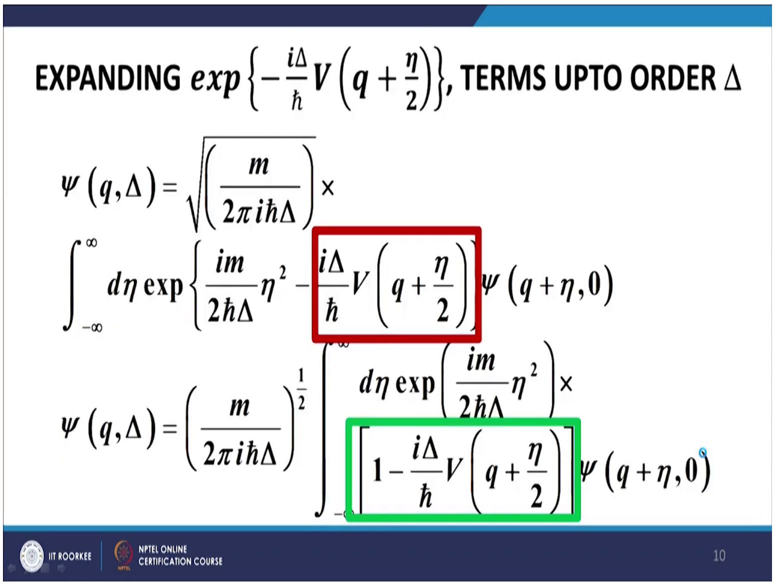

So, the important or the relevant or the dominant contributions are going to come from the area. Now, we expand the potential function also, the exponential of the potential function to first order which is because we are dealing with infinitesimals.

So, expansion to first order is adequate for our purpose and we that is precisely, what we have done in this slide, we have expanded the exponential of i delta upon h bar V q plus eta by 2 as the pre factor remains as it is and we have expanded the exponential as i 1 minus i delta upon h V q plus eta by 2 that is the expansion of this exponential to first order plus of course higher order terms would be there.

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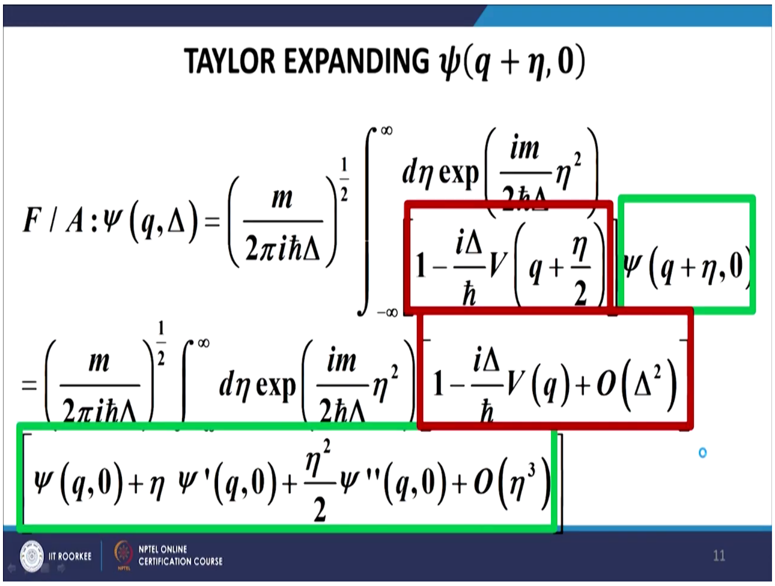

Now, let us expand the wave function as well. When we expand the wave function, this is what we with the red box contains the expression from the previous slide of the expansion of the potential and now, we explain expand the expression in the green box. When we expand the expansion, the expression in the green box, we get the corresponding expression in the green box, in the bottom equation in the last equation. This green box gives you the expansion of psi q plus eta comma 0, it the Taylor expansion around q comma 0.

This is simply the Taylor expansion of q psi plus eta comma 0 around q 0, nothing more Taylor expansion and the rest is same. Of course, we have also expanded this potential function V q plus eta by 2 in terms of a expansion Taylor expansion, V q plus higher order terms higher order terms in eta and this higher order terms in eta would also be multiplied by delta. So, it would be a higher order terms in delta and eta which simply written as order delta square.

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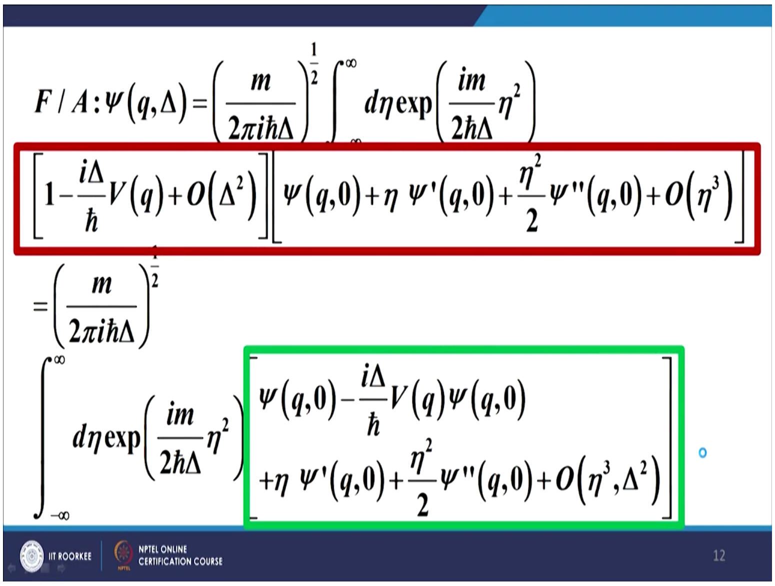

Now, we all we need to do is to simplify the expression given in the red box and to ignore or to eliminate expressions of higher orders that is precisely what is done. If you look at the expression in the green box it is a simple multiplication of the two expressions in the brackets and what we get is the residual part. Of course, the integral the rest of this stuff remains that is as it is and the exponential im upon 2 h delta eta square also remains as it is. The first term as this is this whole thing is to deal with basically the potential term, the simplification of the product of the potential term and the wave function.

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GAUSSIAN INTEGRATIONS

Now, as the integrals have oscillatory integrands, we evaluate them by regularization e.g.

$$\int_{-\infty}^{\infty} d\eta \exp\left(\frac{im}{2\hbar\Delta}\eta^2\right) = \lim_{\delta\to 0+}\int_{-\infty}^{\infty} d\eta \exp\left[\left(\frac{im}{2\hbar\Delta}-\delta\right)\eta^2\right]$$

$$= \lim_{\delta\to 0+}\left[\frac{\pi}{\left(\delta-\frac{im}{2\hbar\Delta}\right)}\right]^{\frac{1}{2}} = \left(\frac{2\pi i\hbar\Delta}{m}\right)^{\frac{1}{2}}$$

Now, we do the Gaussian integrals. If you look at this carefully, this is nothing but a Gaussian integral. The first term exponential im upon 2 h delta upon eta square is a Gaussian integral. We can do it. Of course, we need to adopt a regularization parameter, introduce a regularization parameter, delta here because the integral is oscillatory. So, we introduce a regularization parameter delta and so on simplification; this is what we get.

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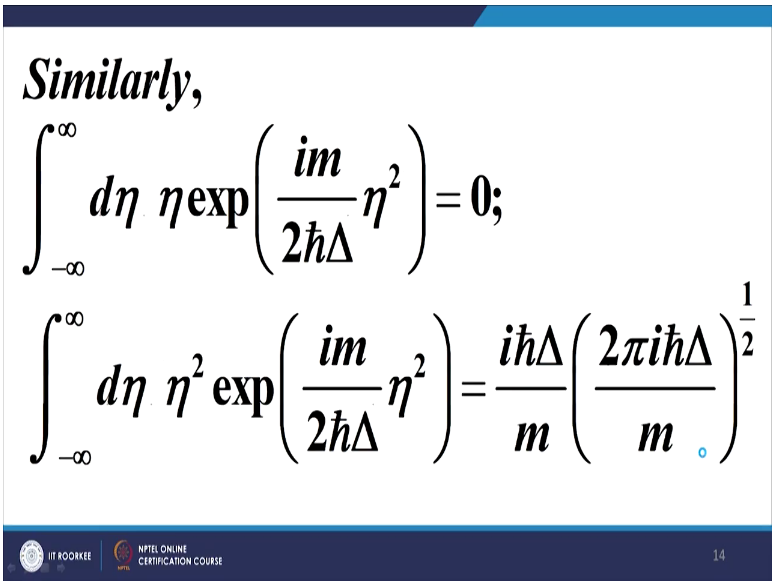

Similarly, we do the integral of eta and it gives us 0 eta exponential im, this expression gives us 0 and the expression eta square exponential im upon 2 h delta eta square integrated over the entire spectrum gives us the expression on the bottom of your slide, right hand side.

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SUBSTITUTE THE GAUSSIAN INTEGRALS

$$F/A:\psi(q,\Delta)=\left(\frac{m}{2\pi ih\Delta}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} d\eta \exp\left(\frac{im}{2h\Delta}\eta^{2}\right)\left[\begin{array}{l}\psi(q,0)-\frac{i\Delta}{h}V(q)\psi(q,0)\\ +\eta\,\psi'(q,0)+\frac{\eta^{2}}{2}\psi''(q,0)+O\left(\eta^{3},\Delta^{2}\right)\end{array}\right]$$

$$=\left(\frac{m}{2\pi ih\Delta}\right)^{\frac{1}{2}}\left[\begin{array}{l}\left(\frac{2\pi ih\Delta}{m}\right)^{\frac{1}{2}}\left[1-\frac{i\Delta}{h}V(q)\right]\psi(q,0)+\\ \frac{ih\Delta}{2m}\left(\frac{2\pi ih\Delta}{m}\right)^{\frac{1}{2}}\psi''(q,0)+O\left(\Delta^{2}\right)\end{array}\right]$$

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Now, we substitute all these values into our original equation. This was our original equation. The top equation was the original equation that we obtained by simplification and we simply substitute the integrals now.

This at the integration has now been done and the integrals have to be substituted. The integral of exponential im upon 2 h delta eta square, then you have eta into this exponential, then you have eta square into this exponential, eta square into this exponential this term. So, all these integrals have been done in the previous slide and we make simple substitutions.

On substituting all these expressions here, what we end up with is given on the next slide. It is here in the green box.

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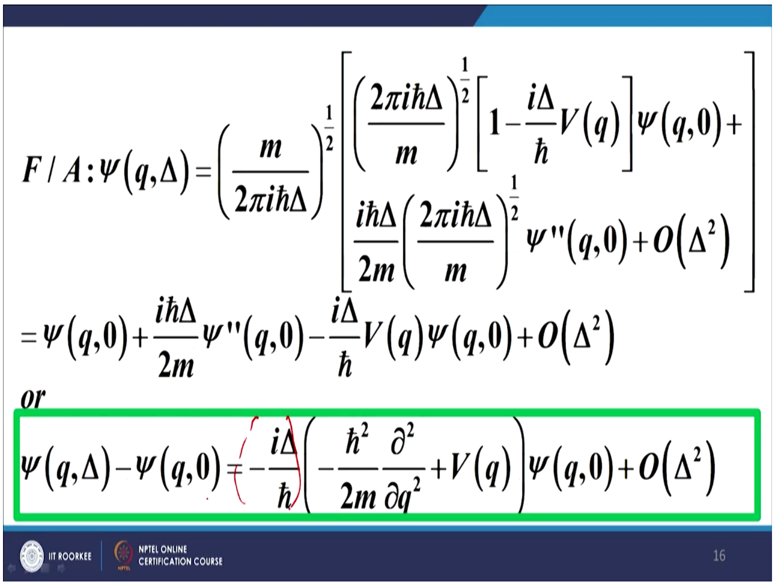

We get psi of q comma delta is equal to psi q comma 0 minus this whole expression. You take psi q comma 0 to the left hand side, you get this expression which is there in the green box right at the bottom of your slide, simple algebraic manipulation; otherwise there is no other mathematical operations and algebraic manipulations and we end up with the expression that is given at the bottom of your slide in the green box.

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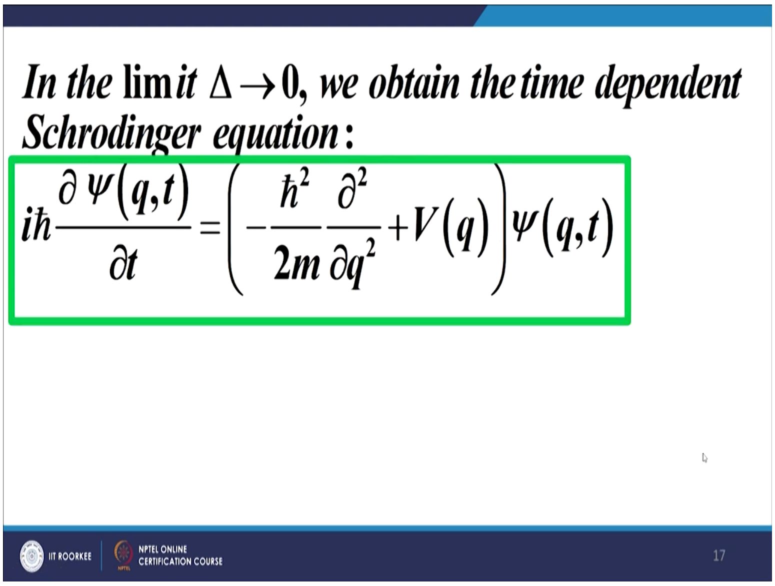

Now, if you look at this, if you if you look at this in the infinitesimal case, if you transfer if you take the limit delta tending to 0, transfer the first of all transfer the pre factor here, transfer this pre factor to the to the left hand side and then, take the limit delta tending to 0. It simply turns out to be a partial derivative of psi with respect to time and that is precisely what is here. Of course, the pre factor becomes ih bar as you can see here.

This minus i upon h bar can be written as 1 upon ih bar because minus 1 is the i square. So, it can be written as i upon i square h bar that is 1 upon ih bar. This goes to the left hand side. It becomes ih bar and delta goes to that denominator, we take the limit delta tending to 0 and we get the i we get ih bar as the pre factor and then, the partial derivative of psi with respect to time and that gives us the left hand side. The right hand side is clearly what we wanted already. If you look at it, it is clearly in the form that we want you ignore the higher order terms and you get the Schrodinger equation.

So, starting from the path integral framework, we have been able to arrive at the Schrodinger equation and that shows clear cut correspondence between the path integral framework and the Schrodinger equation.

So, this is an important nuances important attribute of the path integral framework that there is a correspondence, clear-cut correspondence between the non relativistic path integral and the nonrelativistic Schrodinger equation. Let us now turn to the development of the formalism, development of the formalism of the path integral which will be requiring for the application to quantum field theory.

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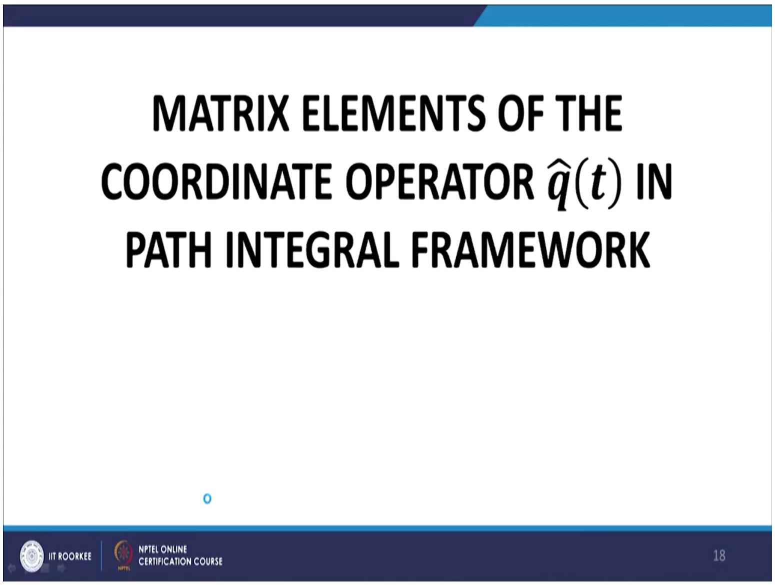

What we do now is to determine the matrix elements of the coordinate operator q hat t in the path integral framework.

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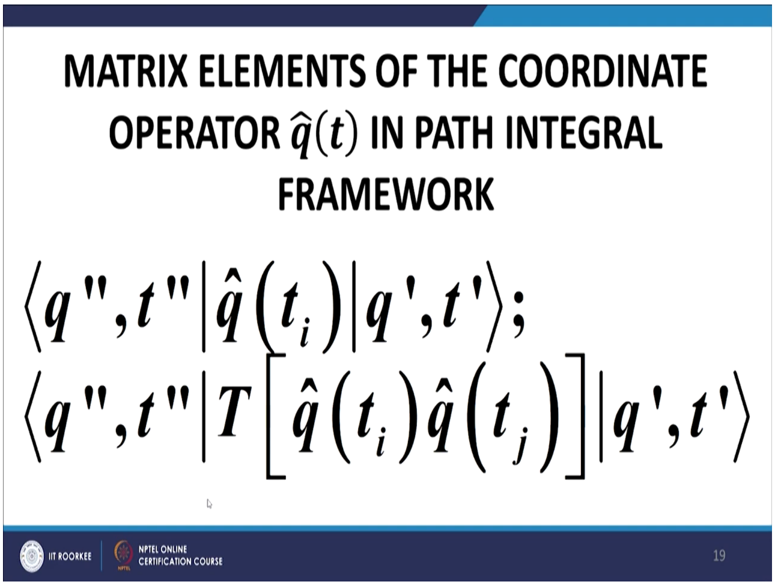

In a sense, what we want to determine is given on your slide. We want to first determine the first expression. The operator q ti at a particular point in time ti stand which between the final state and the initial state and we also want to determine product of such operators stand which between the final state and the initial state of the physical system, quantum physical system in the path integral framework that is our exercise.

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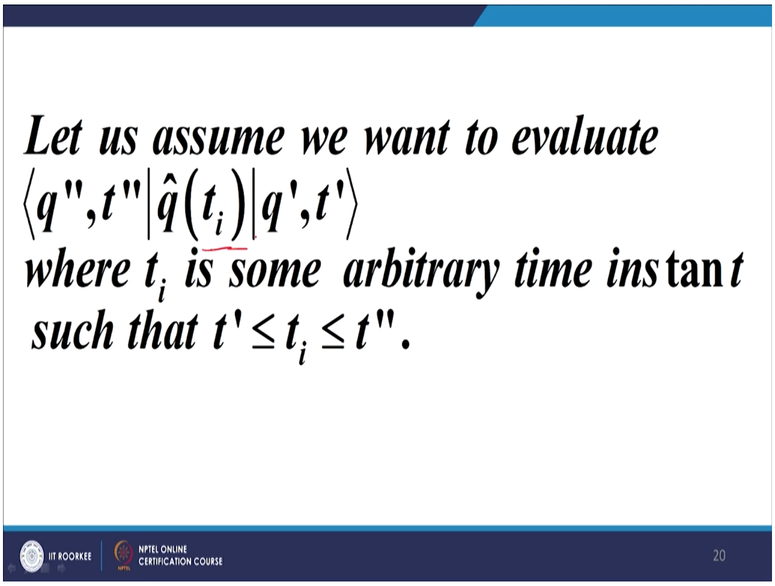

So, let us start with the first problem and the first problem is we want to determine this expression, where ti is obviously, some time interval or some point in time, some point in time between the initial time and the final time.

The time of the starting of the time of this evolution and the up to the final evolution of the system t double dash is the final revolution of this system; t dash it is the initial evolution starting time of the system and ti is somewhere in between, any arbitrary point in between at which you want to observe the matrix element, determine the matrix elements of the operator coordinate operator q which is obviously, time dependent in the Heisenberg framework.

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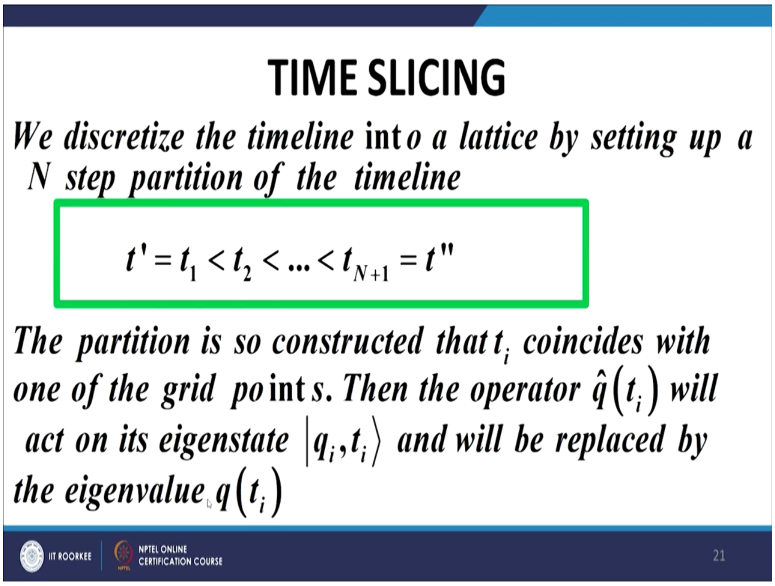

So, what we do is as the we have been doing in fact, we do a time slicing. We discretize the time line into a lattice into a grid and in the form that is given in your green box. The starting time is arbitrary named as t 1 and then, t 2, t 3, these are various points on the time line. Now, the time line consists of a lattice of points a grid of points t 1, t 2, t 3; but while doing so, we have a caveat in mind, we would have a something at the back of our mind that something at the back of our mind is that one of these time points.

One of this discrete lattice points should coincide with the ti at which we were to determine the matrix elements of our given operator. In other words, one of this you see this is a partition of the time line. Now obviously, we have discretion of how to introduce or how to implement this partition, we can make it as fine as we desire.

So, we ensure that the partition is fine enough that one of the points of this partition that is one of the lattice points, one of the nodes of the lattice coincides with the ti that we would not to determine at which we want to determine the matrix elements of the coordinate operator. This particular ti, this ti, this ti should one of should be one of the nodes, one of the points on the lattice or on the grid on in which we have converted the time line. So, having done that, now in then that case in that is obviously possible because we can partition our in our time line into as fine a grid as we like.

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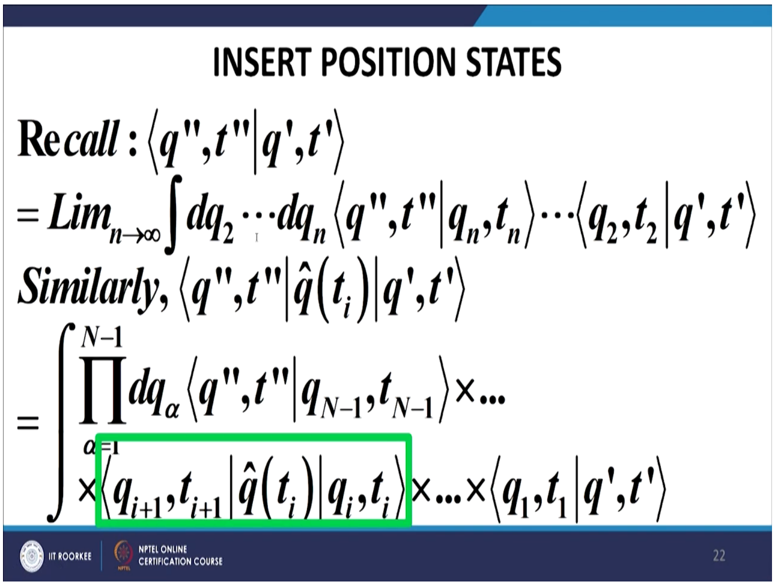

So, that being the case, that being the case what will happen is as you will see later. So, I will come back to it in a minute, but before that what we do is the standard procedure like we had done earlier, when we worked out the path integral, we introduced position, complete sets of position states. We introduced complete sets of position states corresponding to each of those lattice points, each of those grid points as precisely what we have shown in the second integral the bottom equation.

Now, the important point is here because this complete set of states has been introduced and in the moving basis of course, and the one of the grid points, one of the grid points corresponds to over ti. Therefore, at ti also we shall have a complete set of states and which will have some kind of an inner product developed in this form. A sandwich developed between q ti with qi, in this state qi ti on the right. The ket state and the dual state q i plus 1 ti plus 1 on the left. This is precisely, what we will get because of the manner in which we have done the partition.

Now, that being the case, now this operator q ti, this operator q ti will act on the state that is on the right and because you see this state qi ti is the is the eigen state of this particular operator q at ti and therefore, when the operator operates on this particular state, it returns the eigen value of the operator. So, now the eigen value would be a number and therefore, the net effect of this would be to replace this operator q ti with a with a number q ti which represents the eigen value of that operator because of the operation of this operator on its own eigen state.

So, in a nutshell, what we have done is just to recap we have introduced complete sets of states at various time points in the corresponding to the grid and because one of the time points on the grid coincided with the point in time at which we were to determine the matrix elements of the operator. This particular phenomenon happened which enabled us to substitute the operator with its eigen value.

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$$\left\langle q'',t''\middle|\hat{q}(t_i)\middle|q',t'\right\rangle$$

$$=\int\prod_{\alpha=1}^{N-1}dq_\alpha\left\langle q'',t''\middle|q_{N-1},t_{N-1}\right\rangle\times\ldots\times\left\langle q_{i+1},t_{i+1}\middle|\boxed{\hat{q}(t_i)\middle|q_i,t_i\right\rangle}\times\ldots\times\left\langle q_1,t_1\middle|q',t'\right\rangle$$

$$=\int\boxed{[Dq][Dp]q(t_i)\exp\left[\frac{i}{\hbar}\int_{t'}^{t''}(p\dot{q}-H)d\tau\right]}$$

So, what does happen now is as you can see here in the red box, this operator q ti acts on the state qi ti and we get the eigen value q ti. Note this, q ti is without the hat showing that it is a eigen value, it is a number; it is not an operator. And therefore, once this phenomenon is done this q ti can be taken outside this whole sets of states and we will simply what we retain; what we retain is nothing but the original path integral with the expression q ti sandwiched in between as you can see in the green box. The important thing is q ti is now a number, so you can put it here. Because it is no longer an operator and why it is not an operator because of this particular process, whereby we the operator is acting on its own eigen state and returning the eigenvalue.

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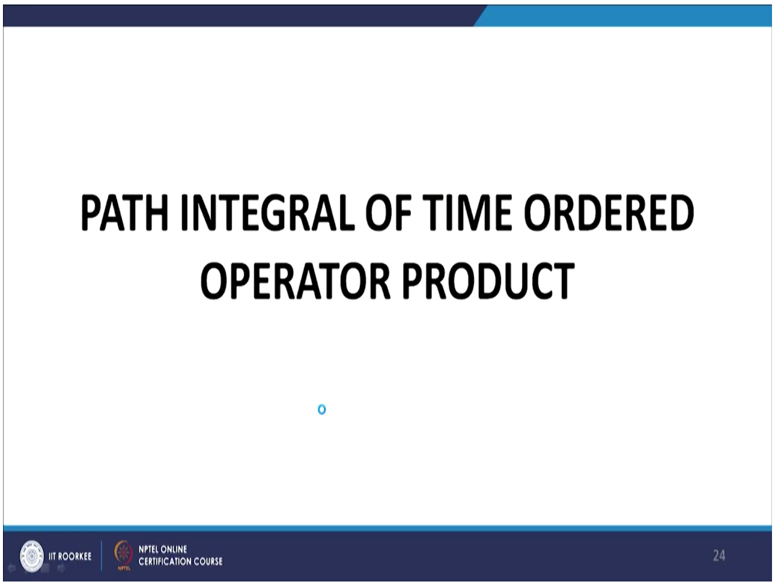

So, that is how we that this is the expression, the green expression is the expression for the matrix element of q operator q ti in the in between the initial state and the final state. Now, we come we develop this formalism further, we now look at the time ordered product operator product of two state of two operators, time ordered product of two operators.

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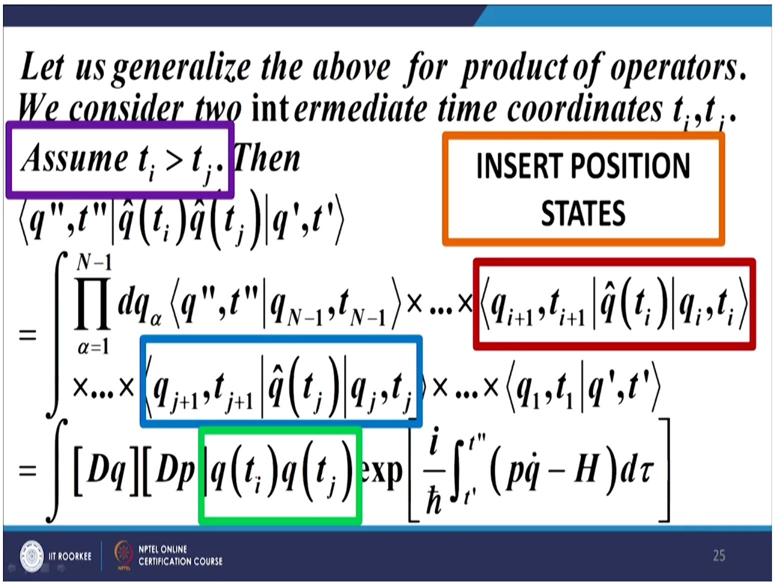

Let us assume that we have got two operators say position operators coordinate operators q ti and q tj. Let us for the moment assume that ti is greater than tj. Let us assume q ti is greater than tj.

Now, as in the previous case, we do the same exercise, we introduce position complete sets of position states; but before, we do introduce complete sets of position states, we discretize the time line as we did in the previous case. Again, we ensure again we ensure that the partitions that we have performed of the time line, the lattice that we have formed of the time line is such that we have nodes corresponding to ti and tj on the lattice.

In other words, these points and these time points corresponding to some nodes on the discretized time lattice or the discretize grid that we have constituted. So, that being the case because we are assuming t i is greater than j, tj or therefore, what will happen is ti will appear to the left and tj will have q ti will appear to the left and q tj would appear to the right as per the on the ordering of the in grid of the lattice.

So, again, what will happen? We will get a situation which is similar absolutely similar to what we had earlier. We will have the operators q ti acting on its eigenstate and at operator q tj acting on its eigenstate because remember these two corresponding correspond to nodes on the timeline. So, both these operators will act on their respective eigenstates and returned with the corresponding eigenvalues.

The net effect is that we can substitute the operators by the corresponding eigenvalues and that is precisely what is done in the green box, the rest of the exercise remains absolutely same and we have the expression for the product or for the matrix elements of the ordered product ordered product.

Which ordered product? q ti q tj sandwiched between the initial state and the final state. The matrix elements of this particular ordered product of operators is given by this expression. Remember q ti and q tj. Now, in the green box are not operators, they are numbers. So, there are they can commute; you can as well write them in the other order. It does not make any difference at this moment. But we will come back to it in a minute.

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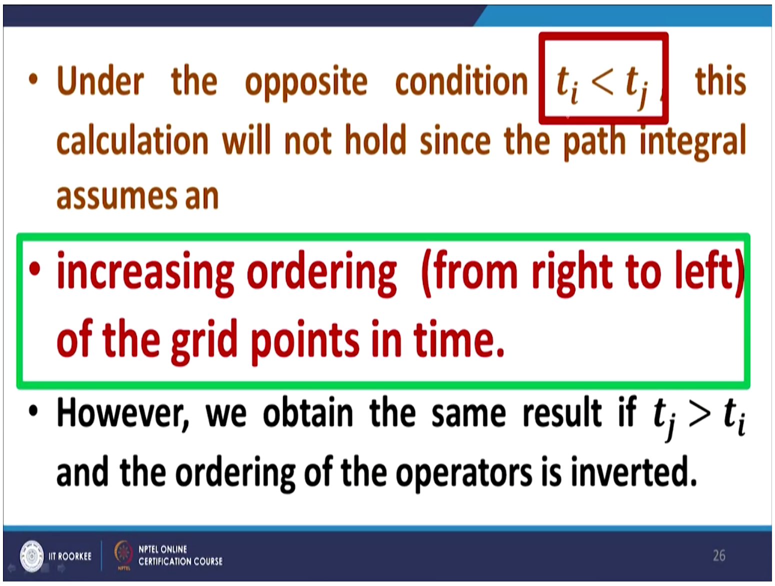

Now, the important thing is suppose this condition t i is greater than t j, we started with the condition. If you recall, we started with the condition that t i is greater than t j, just look at this in the valid box; t i is greater than t j.

Now, suppose we reverse this condition, what happens? Now, if you reverse this condition, then what will happen is that this process that we were able to implement will not be, it will not be possible to implement this particular process. Because in implementing this particular process, we have assumed a sequencing of the states of the timeline rather with the lower with the earlier times being to the left and the later times being to the right.

Timeline moving from the I am sorry, earlier times to the right and later times to the left. As you can see here also ti is appearing to the left and tj is appearing to the right with i ti greater than tj. So, in other words, you are moving from the from the right to the left in terms of the timeline. The gridding or the lattice and numbering is in that form, if the structure of the lattice is such that the nodes initial nodes or the earlier nodes are to the right for and as the node number or the node sequence increases as you move towards the left.

So, this has to be preserved in order that this particular phenomenon takes place and we are able to replace the respective operators with their eigenvalues, this particular ordering has to be respected; otherwise, you cannot do. For example, if qj qj was put to the right and qi qj was put to the left and q i was put to the right, this kind of this kind of placement of the eigenstates would not have been possible and as a result, you could not have replaced them with their respective eigenvalues.

So, this ordering ti greater than tj and the ordering of the operators q ti and q tj must be respected. The later operators must be to the right and the earlier operators or the earlier operators acting at the earlier point in time must be to the to the, I get mixed up, I am sorry. The later operators must be to the left and the earlier operators must be to the right.

You start with the earlier the earliest operator at the at the right hand side and as you move towards the left, time is supposed to increase; time is supposed to increase from the right to the left and if ti is greater than tj, it means what? It means that q ti is occurring after q tj and therefore, q ti would, I would replaced to the left of q tj. So, the important thing is if ti were to be less than tj, then this framework would not work.

And in other words, putting it the other way around, the path integral framework of determination of this kind of matrix elements implicitly assumes a particular ordering. It assumes that the operator that is being placed first is earlier in time, we could place to the right is earlier in time compared to the operator that is placed to the left which is later in time.

It implicitly assumes that it is not withstanding the fact that it is and not explicitly mentioned and if that order is not preserved, then the results would not be consistent. So, under the opposite condition, the calculation would not hold since the path integral assumes an increasing ordering from right to left; right is the lowest, left at the higher of the grid points in time right. So, the conclusions that I have already mentioned.

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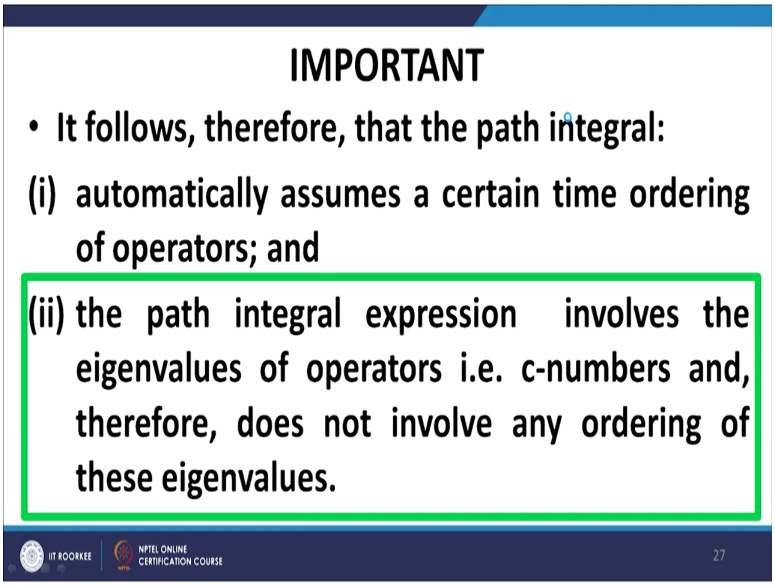

The path integral automatically assumes a certain time ordering from right to left as I said. Right being the earlier, left being the later. The path integral expression involves the eigenvalues of operators. These are c-numbers as I said and they do not involve any ordering, but within that you see the point is once the you put it in the path integral, then the eigenvalues can do commute the eigenvalues being C-numbers, they do not commute.

But their commuting would not influence the order in which the original operators were taken. The odd operators must necessarily be taken with the earlier operator being to the right and the later operator being to the left that has to be preserved. Howsoever, you may write those eigenvalues in the path integral.

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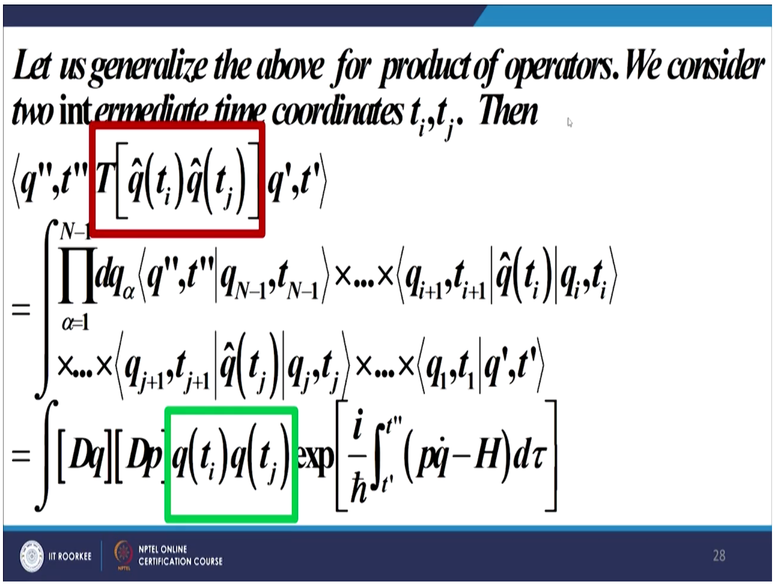

So, this expression can be generalized of course to a number of operators and there is I mean it is a consistent framework. So, instead of having two operators, you can have a number of operators and instead of you know writing time and again that ti is greater than tj. We explicitly, we simply have a time ordering operator placed in front of them which automatically implies that the expression within the square bracket is to be understood in such a way that the earlier operator which so ever it is, the earlier operator is to be taken as the one to the right and the later operator which so ever it is to be taken to the left.

For example, if I write it this way it, you do not have to explicitly see that ti or tj, you do not have to write them explicitly ti is greater than tj. Even if, ti were less than tj; then, writing like this would ensure that q ti appears to the right and q tj appears to the left when you do the actual calculations.

Thank you we will continue from here.