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Lecture - 24 Ground State Expectation Values

Welcome back. So, before the break we derived these two relations which are there on your slide.

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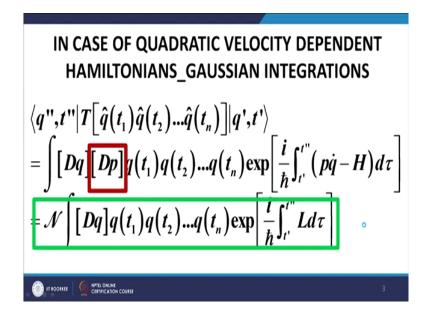
Thus,
$$\langle q'', t'' | T[\hat{q}(t_i)\hat{q}(t_j)] | q', t' \rangle$$

$$= \int [Dq][Dp]q(t_i)q(t_j)\exp\left[\frac{i}{\hbar}\int_{t'}^{t''}(p\dot{q}-H)d\tau\right]$$
and in general:
 $\langle q'', t'' | T[\hat{q}(t_1)\hat{q}(t_2)...\hat{q}(t_n)] | q', t' \rangle$

$$= \int [Dq][Dp]q(t_1)q(t_2)...q(t_n)\exp\left[\frac{i}{\hbar}\int_{t'}^{t''}(p\dot{q}-H)d\tau\right]$$

We derived expressions for the matrix elements in the initial and the final states of time ordered products of operators. Obviously again this can be generalized to more than two operators. We worked it out for two operators; it can be generalized to n number of operators.

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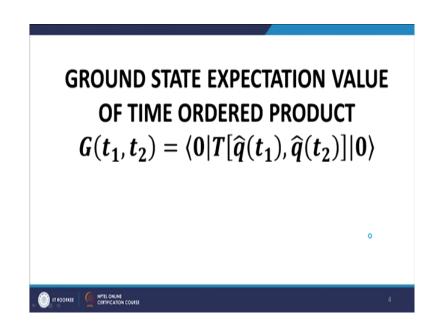


Now, there is a further simplification that can be done in the case of Quadratic Velocity Dependent Hamiltonian. If the Hamiltonian is quadratic in the velocity as we did; as we did in the case of the transition amplitude processes exactly the same.

The path integrals over the momentum space are turned out to be Gaussian in this particular case when there is a quadratic velocity dependence and they can be evaluated explicitly and we are left with expressions in the configuration space. Whereas, you have seen in the green box the Gaussian integrals are captured by the normalization factor and script here and the rest of it is of course to be evaluated in configuration square space.

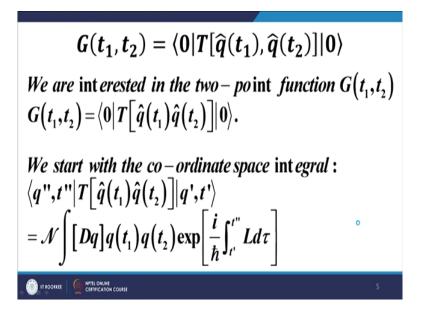
The momentum integrals become Gaussian when there is a quadratic velocity dependent in Hamiltonian and it can be explicitly evaluated, it can be extracted as a normalization factor and the rest becomes simpler to manage.

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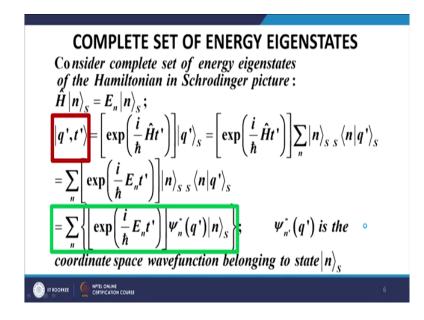
Now, we look at the ground state expectation value of time ordered product. This is a two point function and we want to work out the expression which is given on the right hand side. 0 represent the ground state and the T operator is the time ordering operator which I mentioned before the break and q t 1 and q t 2 are coordinate operators at time t 1 and time t 2 respectively, right.

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So, we want to work out this expression which is given in your slide. What we do is, we start with the coordinate space path integral which is integral for this expression in the initial and final state which the expression for the matrix elements. We start with that and that is given by this in the particular case of quadratic velocity dependence, it is given by the expression which is in the bottom side equation of your slide.

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Now, we put the purpose of further development of this problem. We develop the expressions for the complete set of energy eigenstates and the representation of the wave functions in those bases. The eigenstates are defined by the eigenstates of the Hamiltonian operators.

The energy eigenstates are defined by the eigenstates of the Hamiltonian operator and they are numbered by the respective energy levels. E n is the energy level and the corresponding eigenstate is represented by the ket n. We are working in the Schrodinger picture. The subscript s represents the fact that we are working in the Schrodinger picture.

So, the Hamiltonian acting on the energy eigenstates produces the energy eigenvalue and the energy eigenstates. And let us work out the moving basis q dash t dash. The ket q dash t dash

can be expressed in terms of the evolution operator which is given in the square bracket acting on the; acting on the state coordinate state at t equal to 0.

This is this Schrodinger state at t equal to 0 and this is the state at time t dash. As you know in the Schrodinger picture the states are time dependent and the states evolve with time and therefore, that is precisely what is happening. We are moving from the state at t equal to 0 to the state at q dash t dash by the explicit action of the evolution operator.

Now we introduce in the second step we introduce the complete set of energy eigenstates which is represented by this expression and this one further simplification and the identification of the this product, this dot dot product as the wave function; wave function at q dash corresponding to the energy level n psi subscript n q dash is the eigen function or wave function at q dash corresponding to energy level n belonging to the state n alright.

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$$F / A: |q',t'\rangle = \sum_{n} \left\{ \left[\exp\left(\frac{i}{\hbar}E_{n}t'\right) \right] \psi_{n}^{*}(q') |n\rangle_{S} \right\}; \quad (I)$$

$$Inserting TWO \text{ complete sets of energy eigenstates}$$

$$\langle q'',t'' | T[\ddot{q}(t_{1})\ddot{q}(t_{2})] |q',t'\rangle$$

$$= \sum_{n',n''} \langle q'',t' | n''\rangle_{S} \langle n''' T[\hat{q}(t_{1})\hat{q}(t_{2})] |n'\rangle_{S} \langle n'| q',t'\rangle$$

$$= \sum_{n',n''} \left[\exp\left[-\frac{i}{\hbar}(E_{n''}t''-E_{n'}t')\right] \right\} \psi_{n''}(q'') \psi_{n''}^{*}(q') \times$$

$$= \sum_{n',n'''} \langle n''' T[\hat{q}(t_{1})\hat{q}(t_{2})] |n'\rangle_{S}$$

$$(3)$$

So, this is where we were in the last slide with the first equation was where we concluded the last slide. Now we insert two complete set of energy eigenstates as you first one is shown in the blue box. They are both of them are shown in the blue box. The first one is numbered by identified by n dash priming and the second by a double priming.

So, these are two energy complete sets of energy eigenstates which are inserted as per the boxes given in this equation. Blue box is given in this equation. Now what happens is that these eigenstates in terms of the expression that we had in the first expression that we have the top equation in terms of the top equation, we can write this expression let us call it equation 1 and let us call it equation 2.

In terms of equation 1, we can write equation 2 in the form of equation 3 we have simply, we will simply use the expressions for q dash t dash of equation 1 and simplify the expression for of equation 2 to get equation 3. there is no other change here.

Simply using equation 1 for q dash t dash and q double dash t double dash as well both of them and simplifying them and putting them, we are putting the substituting the kets q dash t dash and the dual q double dash t double dash by the respective expressions on the right hand side. In equation 3, we get this equation 3, right.

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$$\langle q^{\prime\prime}, t^{\prime\prime} | T[\hat{q}(t_{1})\hat{q}(t_{2})] | q^{\prime}, t^{\prime} \rangle$$

$$= \sum_{n',n''} \left\{ \exp\left[-\frac{i}{\hbar}(E_{n''}t^{\prime\prime} - E_{n'}t^{\prime})\right] \right\} \Psi_{n''}(q^{\prime\prime}) \Psi_{n'}^{*}(q^{\prime}) \times$$

$$\sum_{n',n''} \sum_{s} \langle n^{\prime\prime} | T[\hat{q}(t_{1})\hat{q}(t_{2})] | n^{\prime} \rangle_{s}$$

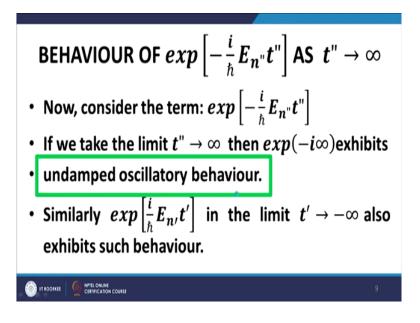
$$We \text{ want to EXTRACT the term with } n^{\prime} = n^{\prime\prime} = 0$$

$$\text{ which gives us } G(t_{1}, t_{2})$$

So, we the expression that we have from above is our first equation. Now the important thing is if you look at this carefully what we want is the expression in this expression we want this expression, but with the condition that n dash equal to n double dash equal to 0, both n the states n dash and n double dash should be the ground state that is what we are looking at.

So, we want to extract this expression with n dash n double dash being 0 that is we want to extract this expression for the ground state. That is the objective from this expression. We have to evolve a mechanism by which you can extract the ground state expectation values.

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Now, let us look at this the some basic behavioral patterns of the functions involved. If you look at the exponential minus i upon h E t or E n double subscript n double dash t double dash at t double dash tends to infinity. This is clearly this expression of itself is oscillatory.

It this represents your oscillatory function in the in the as t double dash tends to infinity. It has a undamped oscillatory behaviour because it is of the form exponential minus i infinity as t double dash tends to infinity. This tends to exponential minus i infinity which has undamped oscillatory behaviour.

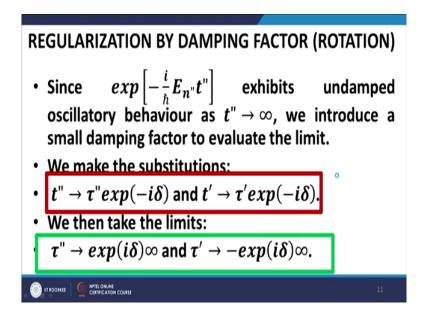
Similarly, for the other exponential i upon h n E n dash t dash in the limit t tends to minus infinity that would also exhibit similar behaviour.

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So, how do we simplify it or how do we extract the ground state from the expression that I mentioned here? From this expression this expression let us call it say equation E. We need to extract the ground state expectation value of t q t 1 q t 2 right. So, we do that by end to invoking the concept of regularization as I mentioned some time back followed by analytic continuation.

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What we do is we introduce a damping factor. You would recall that what I mentioned just now is that this expression in the limit that t tends to infinity is undamped oscillatory behaviour and therefore, it is problematic in computing its integral and as such what we do is, we introduce a damping factor, so that it converges in a sense and at least in the limit t tends to infinity it tends to converge.

What we do, how do we introduce a damping factor? We introduce these substitutions t double dash equals to tau double dash exponential minus i delta. Now this is a damping factor as you will see just now this is a damping factor and t dash goes to tau dash exponential minus i delta.

This gradually yields into the oscillations and as t the time approaches infinity or time increases, the integrals become convergent tau double dash. Therefore, tau double dash can be written as exponential i delta in to infinity in the limit that t tends to infinity.

What happens? Tau double dash tends to exponential i delta in to infinity because this goes to the left hand side, it becomes exponential i delta t double dash. t double dash tending to infinity means tau double dash tending to exponential i delta infinity and similarly for the other case for the case of t double dash t dash.

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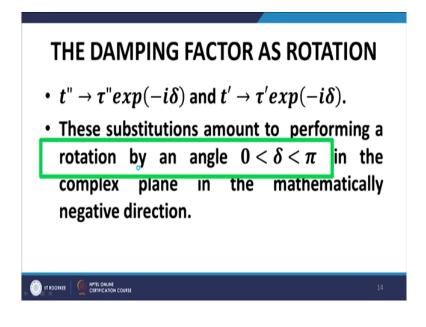
• Now, $exp(-i\delta) = cos\delta - isin\delta$ so that • $t" \rightarrow \tau" exp(-i\delta) = \tau"(cos\delta - isin\delta)$
• $exp\left[-\frac{i}{\hbar}E_{n''}t''\right] \rightarrow$
• $exp\left[-\frac{i}{\hbar}E_{n''}\tau''(cos\delta-isin\delta)\right]$
• = $exp\left[-\frac{1}{\hbar}E_{n''}\tau''sin\delta\right]exp\left[-\frac{i}{\hbar}E_{n''}\tau''cos\delta\right]$
• The first exponential being real converges as $ au'' ightarrow$

Now look at this carefully. Exponential minus i delta can be written as cos delta minus i sin delta. Therefore, t double dash going to tau double dash exponential minus i delta, this is an exponential of how the damping effect is precipitated.

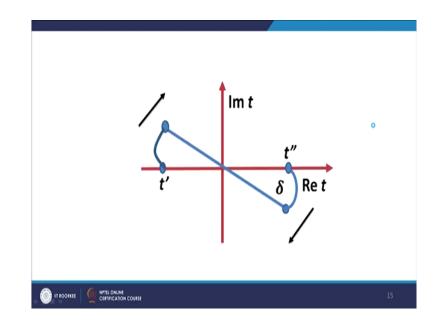
So, t double dash has is substituted by t tau double dash exponential minus i delta and this can be written in this form by substituting the expression for exponential minus i delta. So, exponential of minus i upon h E n dash t n double dash t double dash becomes this whole expression tau t double dash being substituted by tau double dash bracket cos delta minus i sin delta.

Now, the important thing arises. This i and the second term minus i give me a real term and the other term. Of course the cos term remains the imaginary, but we now have a real term to as a pre factor exponential minus 1 upon h; 1 upon h mind you minus 1 upon h E n double dash tau double dash sin delta. Now the first expression being real it converges and it forces the whole integral to converge.

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Now, you can also view this. This is a substitution which is there in the first expression first line, you can also view this as a rotation by an angle of delta in the negative mathematical direction on the in the complex plane.

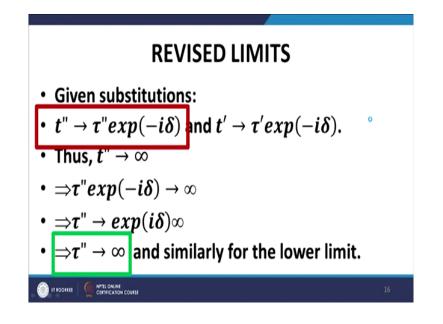


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As you can see here it is a clockwise rotation. Remember we use clockwise rotation in the negative sense and it is a clockwise rotation by an angle delta which you take this real access to the towards the imaginary axis.

So, the damping effect or the damping factor can also be viewed as a rotation by the angle delta 0 less than delta less than pi in the complex; in the complex plane of course and in the clockwise direction, in the negative direction.

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So, we are given this expression. We have made this substitution as t dash tends to infinity. So, tau double dash exponential minus i delta tends to infinity or tau double dash tends to exponential i delta infinity. This implies or here we make an important assumption the concept of analytic continuation.

Here we make the assumption that because this expression is tending to infinity; therefore it should also hold that tau double dash also tends to infinity. This is then this is where the concept of analytic continuation comes in comes into play from the imaginary tau tending to infinity. We are now assuming that tau double dash tends to infinity on the real, this thing real line or real numbers.

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REVISED LIMITS $\left(t_{1}\right)\hat{q}(t_{2})\left\|q',t'\right\rangle$
$$\begin{split} & \left[\hat{q}(t_1) \hat{q}(t_2) \right] \middle| q', e^{-i\delta} \tau' \rangle \\ & \left[\hat{q}(t_1) \hat{q}(t_2) \right] \middle| q', e^{-i\delta} \tau' \rangle \end{split}$$
lim τ " $\rightarrow e^{i\delta}\infty$ NPTEL ONLINE CERTIFICATION COURSE

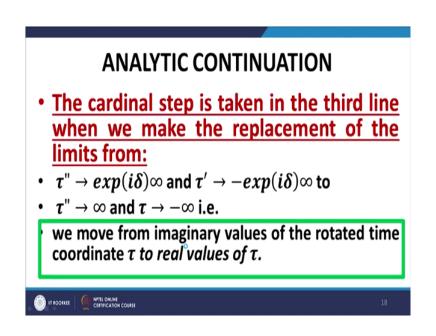
So, what happens to the limits? Now let us look at it very carefully. Remember as you will see later the limits are very relevant in our given problem. You will come to know in the next one or two slides they are very relevant, but for the moment just keep track of the limits.

It is very important you see we are now looking at we basically want to obtain this expression in the limit t double dash tends to infinity t dash tends to minus infinity. You will very soon you will realize that these represent what these will give us the this will enable us to extract the ground state from the expression that I talked about some time back.

So, this is what we want this is what we want now obviously because of the problems we had of the integrals being oscillatory, the exponentials being oscillatory. We could not directly put the limits and extract out the required factors. We adopt indirect procedure. We first in do regularization and then we talk about analytic continuation. The second step is involves the regularization which is nothing, but introducing a damping factor or equivalently introducing a rotation in the complex plane in the negative direction, in the clockwise direction.

Now, this amounts to here we invoke the principle of analytic continuation and we say that if this is the. So, if this is so if the blue box is correct, then the green box must be correct that is what we are in we are assuming by the analytic continuation.

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As I mentioned here highlight here the cardinal step is taken in the third line when we make the assumption, when we make the replacement of the limits from this and this too from the we make the replacement from the limits tau double dash tends to exponential i delta infinity to tau double dash tends to infinity and similarly for the lower limit.

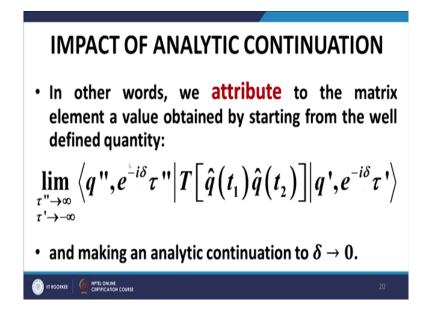
We move from the imaginary values, we move from the imaginary values of the rotated time coordinate to real values. So, that is this is these are imaginary values because of exponential i delta being here. So, we move we assume that if the this holds for imaginary values, it also holds for a real values that continuation from the imaginary values into the real values is where we make the analytic continuation.

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This is admissible mathematically only if the matrix element is an analytic function in the variables t and t'.
Then this transition amounts to analytic continuation.

So, and when is this possible? This is only possible if the matrix elements that we are going to evaluate that the expectation value is an analytic function of t and t dash. So, then this transition this the shift or this as this assumption and amounts to analytic continuation as I mentioned.

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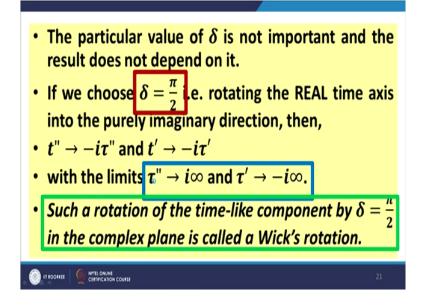
Now, as a result of the analytic continuation whatever we got now, we have got in this situation we the matrix element that we wanted to obtain. No we can attribute a matrix element from you see what we let me explain this. This is a matrix element which is well defined because we have simply made simple substitutions right. Now we assume that there exists a matrix element with the limit with a limit.

Let us go back a minute with these limits; with these limits that is well defined right, but that enables us to define this matrix elements, same matrix element with these limits that is the see look at it.

This is the same matrix element e to the power minus i delta tau double dash. What is this? This is nothing, but t double dash. If you look at this expression, this is nothing, but t double dash. You can look at it here, here it is t double dash is equal to tau double dash exponential minus i delta.

So, these are the substitutions we had made. So this is nothing, but we writing t double dash in a tau double dash, but then we make this a particular assumption that our assumption was the t double dash tends to infinity. Now that implied tau double dash infinity that that implied tau double dash tends to e to the power i delta infinity, but that we assume that implies that tau double dash tends to infinity. So, here we have having this analytic continuation.

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Now, certain clarifications; the particular value of delta that we have chosen you see we never say the delta needs to be small or large or whatever. So, delta is the free. So as long as it remains between 0 and pi, you can take any value of delta between 0 and pi is it is very common to select delta equal to pi by 2.

If you select delta equal to pi by 2, then our substitution original substitution becomes t double dash goes to minus i tau double dash and t dash goes to minus i tau dash and the limits become tau double dash goes to i infinity and tau dash goes to minus i infinity which by analytic continuation remember we said tau double dash goes to infinity and tau dash goes to minus infinity.

Now, this rotation of the you see the real the real timeline into the imaginary timeline by an angle of pi by 2. See that the real timeline of the horizontal line, it is being rotated by pi by 2 to the imaginary line and it is in the clockwise direction. So, it becomes like this and that is what is called a weak rotation.

And, it is very frequently used when we talk about moving from Euclidean path integrals to integrals in Minkowski space. You will be encountering that, it is a very important methodology for handling path integrals because you see the point is path integrals and Minkowski space have certain questions issues of convergence. And therefore, these user practices to work out the path integrals in Euclidean space and then go back to Minkowski space by analytic continuation like we have done just now using Wick rotation.

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Choosing
$$\delta = \frac{\pi}{2}$$
 so that:
 $t' \rightarrow \tau' \exp\left(-i\frac{\pi}{2}\right) = -i\tau' \text{ and } t'' \rightarrow -i\tau''$

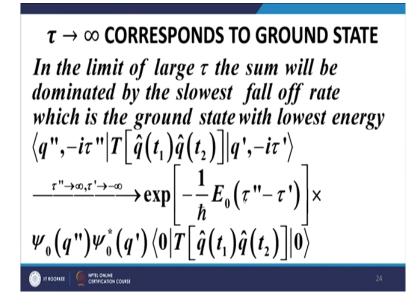
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$$F / A \quad t' \to -i\tau \quad and \quad t'' \to -i\tau'' \\ G(t_1, t_2) = \langle q'', t'' | T[q(t_1)q(t_2)] | q', t' \rangle \\ = \sum_{n', n''} \left\{ \exp\left[-\frac{i}{\hbar}(E_{n''}t'' - E_{n'}t')\right] \right\} \psi_{n''}(q'') \psi_{n''}^*(q') \times \\ G(t_1, t_2) = \langle q'' | -i\tau'' | T[\hat{q}(t_1)\hat{q}(t_2)] | q', -i\tau' \rangle \\ = \sum_{n', n''} \left\{ \exp\left[-\frac{1}{\hbar}(E_{n'}\tau'' + E_{n'}\tau')\right] \right\} \psi_{n''}(q'') \psi_{n''}^*(q') \times \\ = \sum_{n', n''} \left\{ exp\left[-\frac{1}{\hbar}(E_{n'}\tau'' + E_{n'}\tau')\right] \right\} \psi_{n''}(q'') \psi_{n''}^*(q') \times \\ F(t_1, t_2) = \langle q'' | T[\hat{q}(t_1)\hat{q}(t_2)] | n' \rangle_{S} \right\}$$

So, this is the substitution that we did. Now by doing this substitution what do we have now? If we go back to where we started then we have G t 1 t 2. This is the matrix element in the initial and final states and when we simplify this expression, you get q double dash here and instead of using delta equal to pi by 2 we can write this as minus i tau dot t double dash as minus i tau double dash and t dash as minus i tau dash.

So, that is the expression is taken here and if we write this expression, here also substitute the expression for t double dash and t dash in the prefactor also the i factor clubs with this i factor earlier and I get a factor of 1 here. So, this is simply algebraic simplification.

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Now, the important thing that thing that, I mentioned earlier that why we need to extract. This states with t equal to or t double dash equal to infinity and t dash equal to minus infinity. The important point is that the sum that we have talked about this the sum that we have talked about just now in this on the previous slide in this particular sum as time passes, the state that would remain is as time tends to infinity as the time of evolution tends to infinity, the state would remain that would make the most dominant contribution in the situation.

The state that would remain in the situation that makes the most dominant contribution when time tends to infinity would be the ground state because ground state has the least energy. So, having the least energy as a result of which as time tends to infinity, the one state that will make the maximum contribution in the situation when in an infinite time is elapsed would be the ground state. Why? Because it has the lowest energy and therefore, its fall the fall off rate of this ground state is the least because it has the lowest energy.

So, naturally the fall off rate or the loss of energy from the ground state would be the least and therefore, when you take the limit as t tending to infinity, the state that remains is nothing, but the ground state. So, in other words what we want to extract from this is the ground state.

In other words as I take the limit tau double dash tending to infinity tau dash tending to infinity what I get is what I want that is exponential minus i 0. This expression from which I can clearly extract out this particular factor, this is what is required the expectation value of the time order product of operators q t 1 q t 2.

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$$From \langle q'', -i\tau'' | T[\hat{q}(t_1)\hat{q}(t_2)] | q', -i\tau' \rangle$$

$$= \sum_{n',n''} \exp \left[-\frac{1}{\hbar} (E_{n''}\tau'' - E_{n'}\tau') \right] \Psi_{n''}(q'') \Psi_{n''}^{*}(q')$$

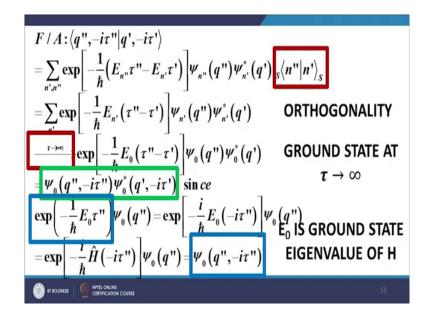
$$= \sum_{n',n''} \exp \left[-\frac{1}{\hbar} (\hat{q}(t_1)\hat{q}(t_2)) \right] | n' \rangle_{S}$$
we also have,
$$\langle q'', -i\tau'' | q', -i\tau' \rangle$$

$$= \sum_{n',n''} \exp \left[-\frac{1}{\hbar} (E_{n''}\tau'' - E_{n'}\tau') \right] \Psi_{n''}(q'') \Psi_{n''}^{*}(q') s \langle n'' | n' \rangle_{S}$$

So, the my problem is now to take the limits or to get the limits in the situation that t tau tends to infinity tau double dash tends to infinity. I am sorry and tau dash tends to minus infinity.

So, this is the this is what we had from above. So, no problem with that and as far as the dotting of these two states are directly concerned without the matrix elements we get this expressions straight away n double dash n dash, these two factors would not make their presence, would not make their appearance. Now the important thing is we look at this expression.

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You look at this expression we can simplify it considerably by invoking the orthonormality of the energy eigenstates and the n double dash equal to n dash survives, the rest of the states go away and we have the summation over n dash only and the n double dash quantity simply goes away.

Now, in the limit that tau tends to tau dash tends to infinity tau double dash tends to infinity tau double dash tends to infinity tau dash tends to minus infinity. What happens? We get this particular expression. This is the expression that we had for the ground state, why?

That is as shown here;

this expression amounts to the application of the simultonian on this wave function and that is simply this particular state. How? So, to repeat how I have got the expression in the green box is shown by how by the expressions in the blue box right. Recall that e 0 is the ground state eigenvalue of the Hamiltonian. So, that has been used in arriving at the ground state wave function. (Refer Slide Time: 27:08)

$$Hence, \langle q^{"}, -i\tau^{"} | T \left[\hat{q}(t_{1}) \hat{q}(t_{2}) \right] | q^{'}, -i\tau^{'} \rangle$$

$$\xrightarrow{\tau^{"} \to \infty, \tau^{'} \to \infty} \exp \left[-\frac{1}{\hbar} E_{0}(\tau^{"} - \tau^{'}) \right] \Psi_{0}(q^{"}) \Psi_{0}^{*}(q^{'})$$

$$\langle 0 | T \left[\hat{q}(t_{1}) \hat{q}(t_{2}) \right] | 0 \rangle \right] - \langle t \rangle$$

$$and \langle q^{"}, -i\tau^{"} | q^{'}, -i\tau^{'} \rangle$$

$$\xrightarrow{\tau^{"} \to \infty, \tau^{'} \to \infty} \exp \left[-\frac{1}{\hbar} E_{0}(\tau^{"} - \tau^{'}) \right] \Psi_{0}(q^{"}) \Psi_{0}^{*}(q^{'})$$

$$= \Psi_{0}(q^{"}, -i\tau^{"}) \Psi_{0}^{*}(q^{'}, -i\tau^{'}) - \langle t^{'} \rangle$$

So, at the end of the day what do I get in the limits that tau double dash tends to infinity tau dash tends to minus infinity. I get this expression on the one side, this is equation 1 and I get this expression, this is equation number 2.

Now, as you can see here the first the prefactor of the quantity that I require the prefactor of the quantity that this is the quantity that I require, the prefactor of this that is this whole quantity is nothing, but this expression which is nothing, but this expression. So, let me repeat the prefactor of the quantity that is required in equation 1 is the same as the quantity in equation 2.

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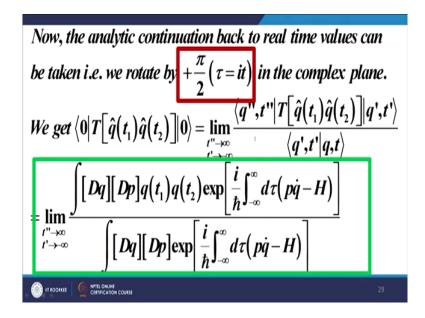
$$Thus, \langle 0 | T[\hat{q}(t_1)\hat{q}(t_2)] | 0 \rangle$$

$$= \lim_{\substack{\tau'' \to \infty \\ \tau' \to -\infty}} \frac{\langle q'', -i\tau'' | T[\hat{q}(t_1)\hat{q}(t_2)] | q', -i\tau' \rangle}{\langle q'', -i\tau'' | q', -i\tau' \rangle}$$

$$\langle \mathbf{w}$$

So, that enables us to isolate the quantity of interest and present it as the expression in the green box.

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So, now the last step is to do the analytic continuation back. We earlier we had the analytic continuation from with an angle of pi by 2 clockwise. Now, we revert pi by 2 counter clockwise and using that we go back to our original variables t dash and t double dash and write the integral as t double dash tending to infinity t dash tending to minus infinity of this expression.

So, and which in the path integral framework we arrive at as the expression in the green box. So, the expression in the green box limit t double dash tending to infinity t dash tending to minus infinity of the path integral numerator path integral denominator numerator. We have the additional quantities or the eigenvalues of the two operators gives us the; gives us the vacuum state expectation value of q 1 and q 2 time ordered. Thank you.