Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
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Lecture 28
Reyleigh Schrodinger perturbation Methods and Adiabatic Switching

Greetings, so we did the Gell-Mann and Low theorem in our previous class and we obtained a certain expression with reference to the adiabatic switching technique which we introduced in the previous few classes we have discussed this. We will also examine how it corresponds to the Rayleigh Schrodinger perturbation formalism.
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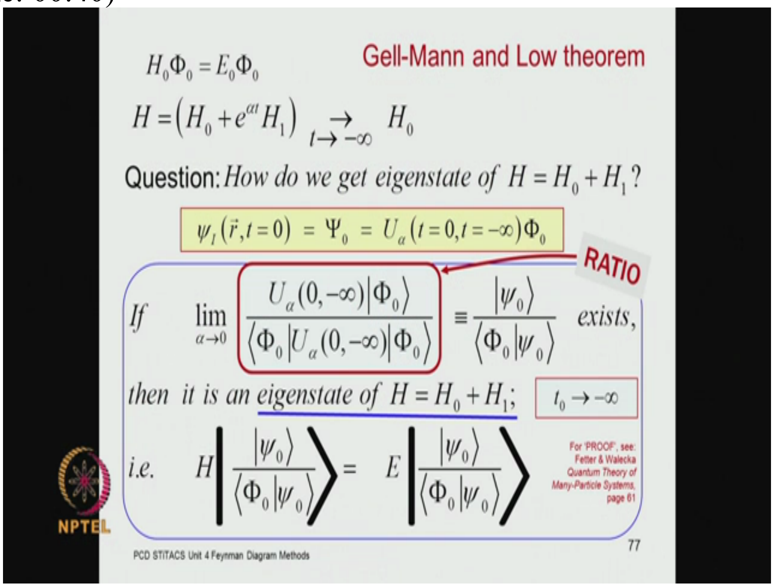

So, this is the Gell-Mann and Low theorem just to remind you a few things that we did in our previous class, so that we quickly recapitulate on that and then take it from there. Our question is that if we introduce a artificial mathematical parameter alpha with which we control the correlation or part of the Hamiltonian which you are not able to handle using normal methods of quantum theory for which you need some special techniques.

So, alpha is this control parameter and our interest of course is in getting the Eigen states of the full Hamiltonian. The Eigen state of the full Hamiltonian actually will come down to the Eigen states of the unperturbed Hamiltonian as t goes from minus infinity because e to the minus alpha t will kill the H1 term as t goes to minus infinity okay.

And then as t goes to 0 you have the full Hamiltonian which is H0 + H1 that is the problem in which we are interested. And we are trying to ask this question that if we know the Eigen states of the unperturbed Hamiltonian how do we get the Eigen states of the full Hamiltonian inclusive of the complexity which is there in the full Hamiltonian.

So, we found that in the interaction picture the wave function at t = 0 can be obtained from the Eigen state of the unperturbed Hamiltonian Phi 0 through this time evolution operator. But then we carry a subscript alpha on this because the time evolution will depend on how you are turning on the perturbation.

So, we are a little specific about this and our final results of course would be independent of alpha. And the Gell-Mann and Low theorem tells us how such an Eigen state can be obtained it tells us that if this limit exists the limit of the ratio, the limit as alpha tends to 0. And it does not worry about whether the limit of the numerator and the limit of the denominator exist independently.

They may have certain divergences which may cancel each other. But then if this ratio has got a well-defined limit then the Gell-Mann and Low tells us this theorem tells us that it will be an Eigen state of the full Hamiltonian.
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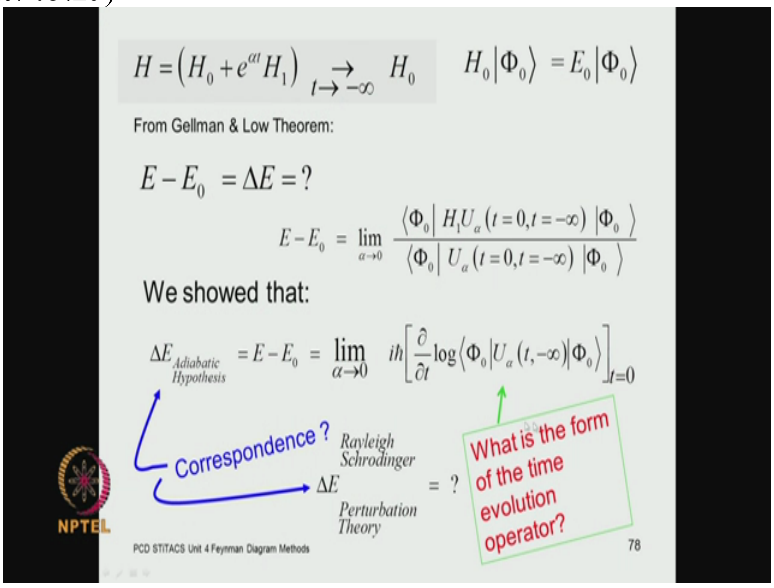

So, we discussed some aspects of this theorem and using that we showed that it tells us what the energy difference will be between the energy of the full Hamiltonian Eigen state, the Eigen value of the full Hamiltonian and the Eigen value of the unperturbed Hamiltonian. So, there is a certain energy difference and using the Gell-Mann and Low theorem we showed that this energy difference; this is the correction which we get okay.

And we also showed using algebraic methods that this particular ratio in the limit alpha going to 0 turns out to be equal to limit alpha tending to 0 and then it is a limit of what it is the limit of the time derivative of the logarithm of this matrix element. The time derivative taken at t =

0, then of course there is this you know ih cross scaling which we have already discussed. So, these are some of the things that we did in our previous classes.

And the question that we had raised is what would be the correspondence of the delta E correction that we get from the adiabatic hypothesis with the corresponding correction from the Rayleigh Schrodinger perturbation theory which is our usual idea of getting corrections when we are not able to solve a quantum mechanical problem fully.

So, we solve a part of it which is the unperturbed Hamiltonian and then we make a correction which is the perturbation. So, this will be examined in the context of what is the nature of this time evolution operator what exactly is the form of this time evolution operator and that is something that we have already discussed in our previous classes.

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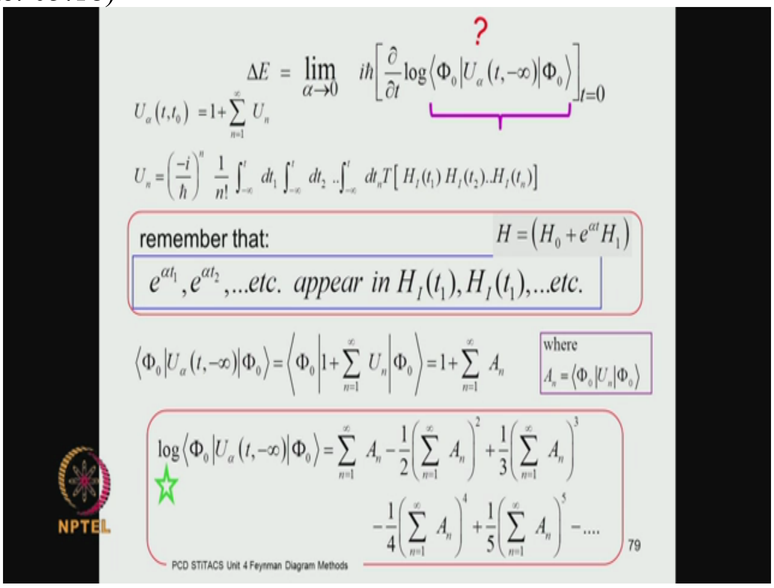

So, let me quickly recapitulate some of those expressions here. So, this is the time evolution operator and we are inquiring what it is. So, we have earlier expressed it as an infinite series okay from n = 0 to infinity. The term corresponding to n = 0 is just the unit operator and then you have the rest of the summation which is from n = 1 through infinity of Un.

And each Un is given by a number of terms in which there are the interaction picture Hamiltonian appears n times with n different time arguments but then notice that there is this chronological operator over here which ensures that all the latest operators in time appear farthest to the left. So, that is the time ordering that is involved in the expression for Un.

Now HI t1 which and whenever you consider this please always remember that it will also include this e alpha t parameter because that is a mathematical you know factor that you have inserted and the time argument t which we wrote generally as t will be different in each case because this is a HI t1. So, there will be an alpha t1 corresponding to this there is an HI t2 over here so there will be an e alpha t2 corresponding to this.

So, all of these terms will have to be carried over very carefully okay. So, now let us first look at this matrix element which is a matrix element of the time evolution operator in this unperturbed state of the Hamiltonian, so this is what it is. And this time evolution operator is 1 + this sum from 1 through infinity of Un.

And from the first term you just get the scalar 1 and then you get An, which is our abbreviation for the matrix element of Un in the unperturbed Eigen value of the Eigen value of the unperturbed Hamiltonian. Now subsequently how to take the logarithm of this and this being the small quantity you can expand this logarithm and we discuss this as well in our previous class that the logarithm of this turns out to be given by this expression.

And now you understand why I used an abbreviation An for this matrix element because the number of terms already fill up the space for us to write the expression and if you keep writing the entire matrix element it is just too much to write. So, this is some sort of a compact notation that we are developing and we have to keep track of what is what.

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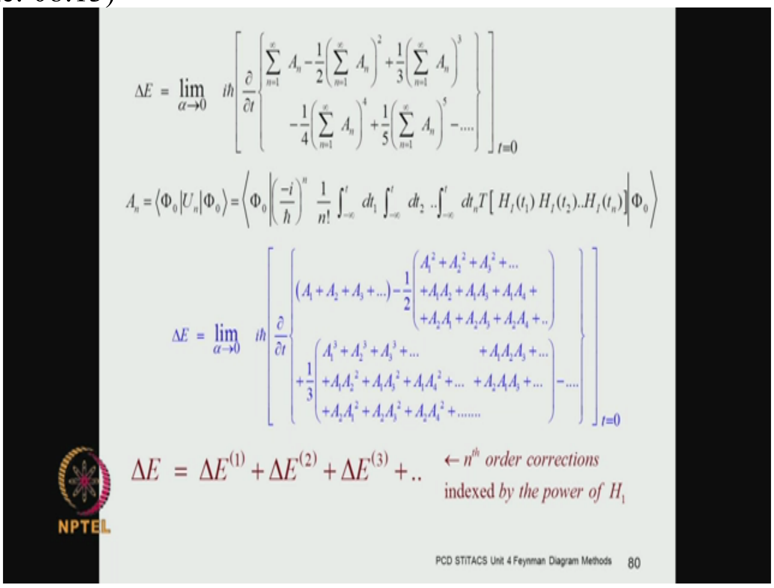

And we have a fairly complex expression over here because the energy correction now will be the time derivative taken at t = 0 of the logarithm expansion and you have got a number of terms over here. Each An itself is quite a complicated factor it has got n different time integrals over different time domains. And if you expand these terms summation over An from n going from 1 through infinity you have A1, A2 and so on.

Then you have got the squares of this then you have got the cubes of this and when you take the squares and the cubes and so on notice that you get A1 square you also get A1, A2 you will also get A2 A1. When you take the cubes you will not only get A1 cube, A2 cube, A3 cube, you will also get A1, A2, A3. Then you will get A2, A1, A3 in different orders and these are all operators, so their positions are very important okay.

And in general the energy correction can be obtained into different orders depending on how many times the interaction appears in the operator whose matrix element is under consideration okay. So, there are nth order terms that you can get and this is really quite complicated, you see that these terms come from a variety of combinations of A1, A2 and A3 and in multiple different orders. When you go to even higher order terms it becomes that much more complicated.

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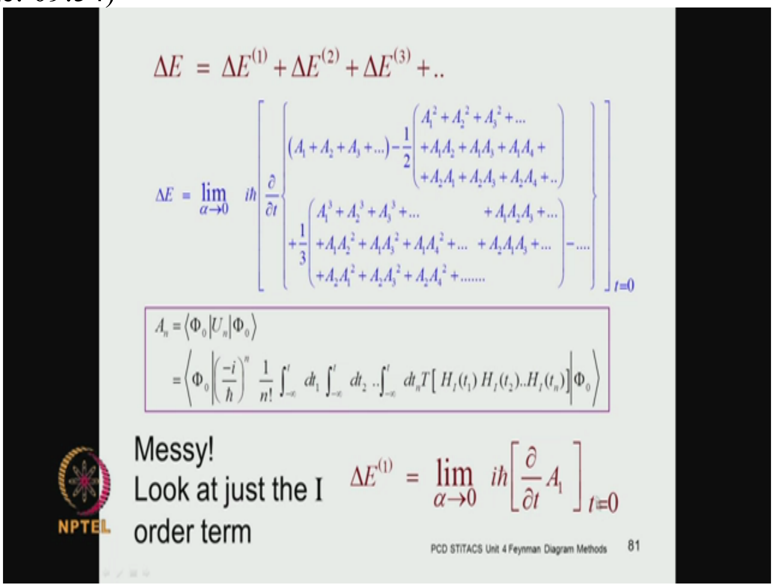

So, it is quite a complex kind of mathematical system of equations that we have to work with. And to get familiar with the techniques we will first work only with the first order terms just to see how; that because that is the simplest that you can work with. And the first order correction to energy would then be given by limit alpha going to 0 ih cross del by del t.

And only the first order term we take del by del t of this A1. And this time derivative of course has to be taken at t =0. So that is the first order term that we shall consider.

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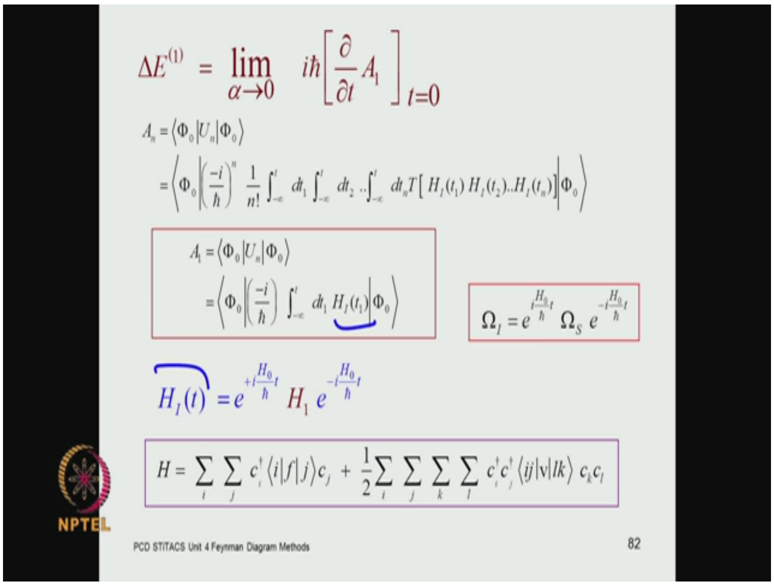

So, now let us see how we can work this out now this is the general expression for An for an arbitrary value of n. So, for a particular value of n which is n = 1, we have this expression and now there is only one time integral over here okay. HI appears only once with a dummy label which gets integrated out the dummy label is t1 okay. The limits of integration are from minus infinity to t okay.

Now in general you can carry out the transformation from a Schrodinger picture operator to an interaction a picture operator using this prescription which is the general expression. So, you can get this HI this is the interaction picture Hamiltonian for the interaction by carrying out a transformation on the Schrodinger picture operator H1 by carrying out this transformation e to the IH 0 over h cross t H1.

And then you have e to the minus Ih 0 H cross t, so you are just applying this rule over here. But you can plug in the explicit form of H1 which we already know in the second quantized form which we have done in great details in one of our earlier units okay. The unit on in the unit on second quantization we wrote the n electron Hamiltonian in the second quantized creation and destruction operators, so we will use this form.

So, this is what H1 is, however it is H is a little bit more than that because this is the raw H1 but then we have introduced this adiabatic switch mathematical factor e to the alpha t. So, in addition to that you will have this e to the alpha t factor okay. So, that is something that you have inserted as a mathematical device.

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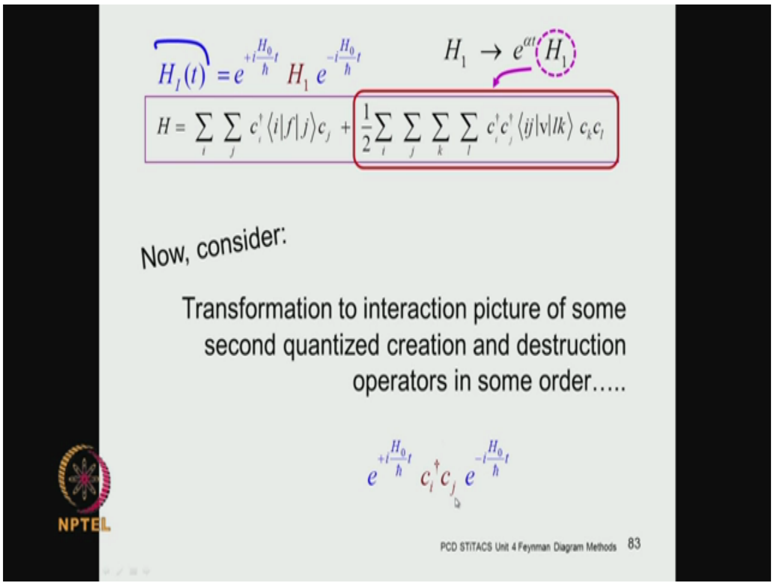

So, this is your H1 along with this e to the alpha t and we have to carry your transformations of this operator to the interaction picture. So, we will have to carry out transformation of all these creation and destruction operators somewhere over here, it comes as ci dagger cj here, it comes as ci dagger cj dagger if you look at this, this would be ck, cl. So the creation and destruction operators will come in a variety of different combinations.

Because you are also summing over all of these i, j, k and l indices over here and i and j indices over here, so they will come in a variety of combinations and we will and it does not matter in what order they come. So, we will take any one of them just to see how the creation and destruction operators transform to the interaction picture. So, we will consider just one such combination which is ci dagger cj.

There is nothing particular about particularly important about it, it is just some set of two operators and we will see how they transform to the interaction picture. So, sure enough they will be ah they will be sort of sandwiched between e to the iH0 t and e to the - i H0 t and this is how they will transform. So, let us examine this term over here okay.

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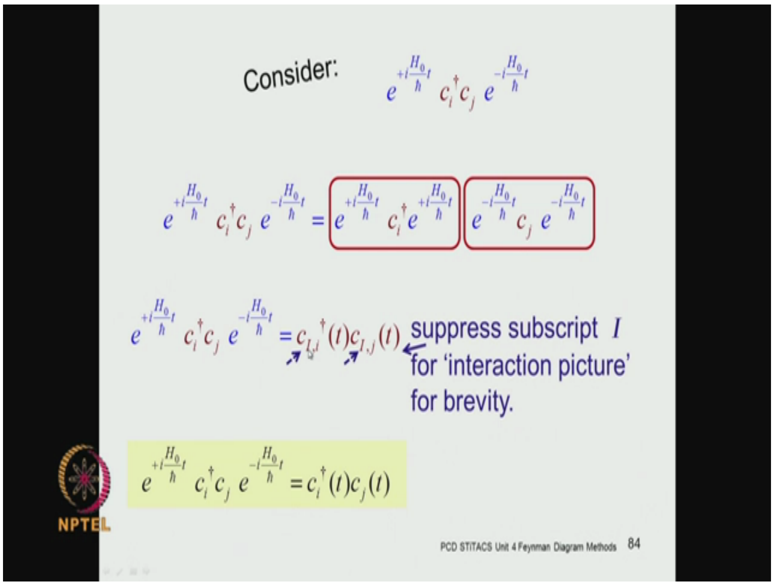

So, this is the term we are going to examine now what do we find here, in between this these two operators creation and destruction operators you can always plug in a unit operator. So, this is the unit operator which has been plugged in and now using the associative law you find that these three operators give you the transformation of ci dagger to the interaction picture.

And these three operators give you the transformation of cj to the interaction picture right. So, what do we get, we find that this combination of operators transforms to the interaction picture and what you get is the same kind of an operator. So, here you have ci dagger and cj here also you have got ci dagger and cj but there is this subscript i which tells us that this is now in the interaction picture okay.

So, the general form is retained but these are different operators they are the operators in the interaction picture and just for the sake of brevity because of our notation is already complicated now that we know that we have carried out this transformation to the interaction picture.

We have the time argument explicitly indicated in the parenthesis; we know that these are interaction picture operators. So, I will suppress the subscript i and always I will remember that ci dagger t is an interaction picture operator okay. Because those are the ones which are time dependent. So, I will suppress the notation the subscript i will be notation in subsequent analysis.

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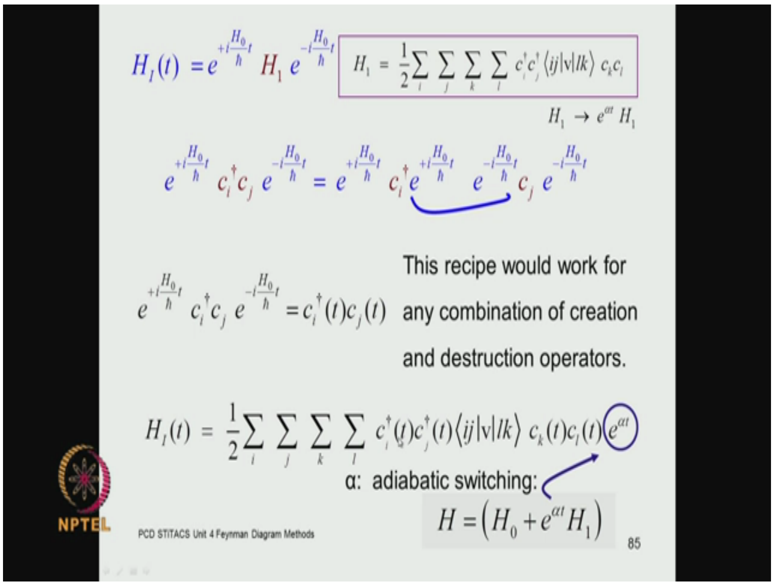

So, this is the operator that we have to transform to the interaction picture along with this e to the alpha t. So, you have the transformation to ci dagger or cj t and now all of these operators ci dagger goes to ci dagger t cj dagger t cj dagger over here goes to cj dagger t in the interaction picture same thing with ck and cl, so ck goes to ckt and this cl goes to clt and we have this e to the alpha t coming in over here okay.

So, now this is our interaction picture Hamiltonian corresponding to the two electron terms. So, these are the terms which we had difficulty with and this is the one which corresponds to the difficult part which you cannot solve using ordinary quantum mechanics. With ordinary quantum mechanics you can only solve part of the problem which is H0, H1 is the difficult part.

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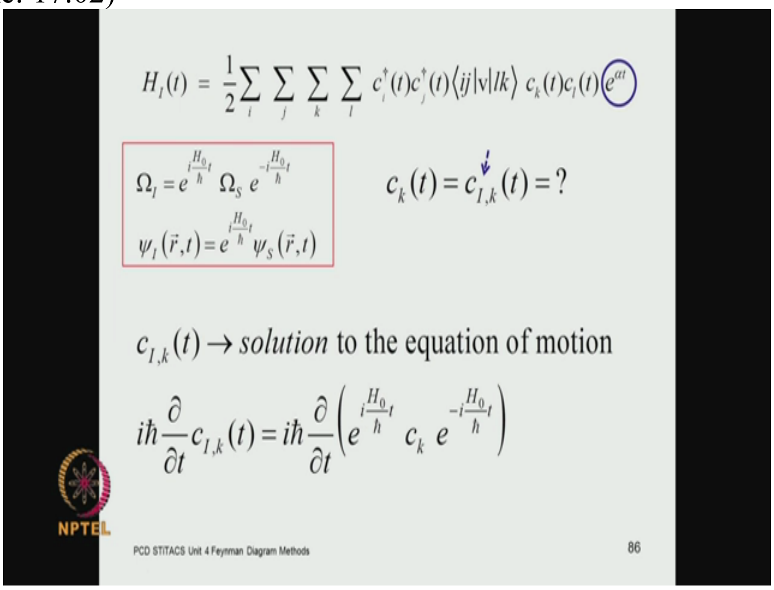

So, this is the interaction picture two electron terms okay. Now let us ask what is the explicit form of this operator ck in the interaction picture okay this is already in the interaction picture this is the index subscript that we are suppressing and we are asking what is the explicit form of this annihilation operator because it will be a solution to the equation of motion for the annihilation operator right.

So, the equation of motion for the annihilation or the destruction operator is this which is ih cross del over del t of ci t, but ci t is nothing but an operator which is obtained in from c, this is ck actually right. So, ck is ckt is the operator that you get in the interaction picture from the corresponding Schrodinger picture operator.

By these transformation operators according to the general prescription of getting an interaction picture operator from the Schrodinger picture operator. So, this is the equation of motion kind of thing this is the time derivative of c and this tells us its solution will give us the explicit form of c.
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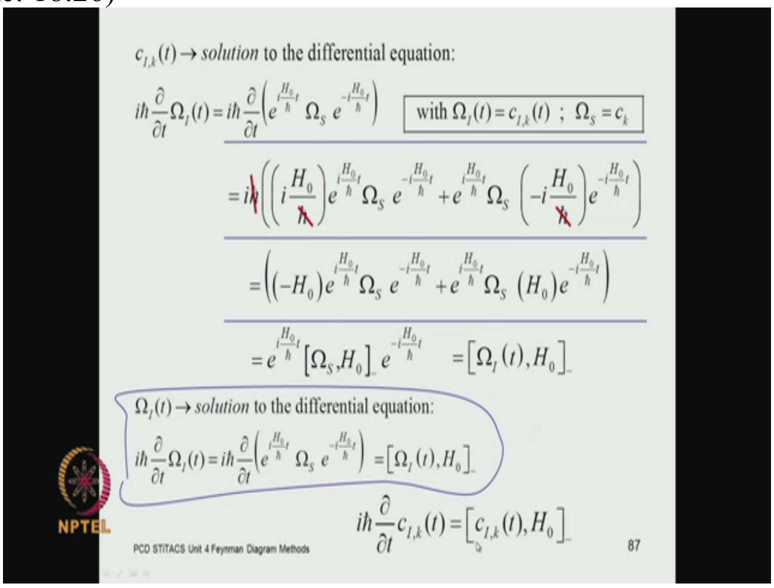

So, let us work this out so this is the time derivative of a product of these three operators okay of which omega s is not time dependent but this one is and so is this. So, if you take the partial derivative with respect to time and do it term by term but when you do so make sure that the order of these operators is retain because you cannot assume that any pair of this automatically commutes okay.

So, you have to keep track of the order, so from the first term you get is iH0 over h cross when you take the time derivative. Then you have got these three operators and then omega s is not dependent on time but then you have to take the time derivative of this which is -i H0 over h cross and then you have got this operator okay. So, if you just rearrange these terms you can get rid of the h cross which cancels very nicely.

And you can rearrange these terms you have got i here and i here. So, i square will give you - over here, so you have this term omega H0 with a plus sign and you have got -H0 omega okay. Here you have these two operators in the reverse order but with a -sign this H0 of course commutes with e to the iH 0 over h cross okay.

So, if you just rearrange these terms you find that you have got the commutator of the Schrodinger picture operator commutator with the unperturbed Hamiltonian sandwiched between these transformation operators, so that is the results that you get okay. So, this is nothing but omega i t which is the interaction picture operator corresponding to the Schrodinger picture operator omega s.

So, that is what you get because H0 of course commutes with e to the iH 0 and also with e to the –i H0 these are expansions in powers of H0. So, to get omega i you have to solve this equation which is the time derivative of omega i is then given by the commutator of omega i with H0 this is valid for any operator omega and therefore it will be valid also for the destruction operator in which we were interested.

So, the time derivative of the destruction operator will be given by the commutator of the destruction operator with H0. Now this is what we can easily determine because we know H0 in terms of the creation and destruction operators okay.

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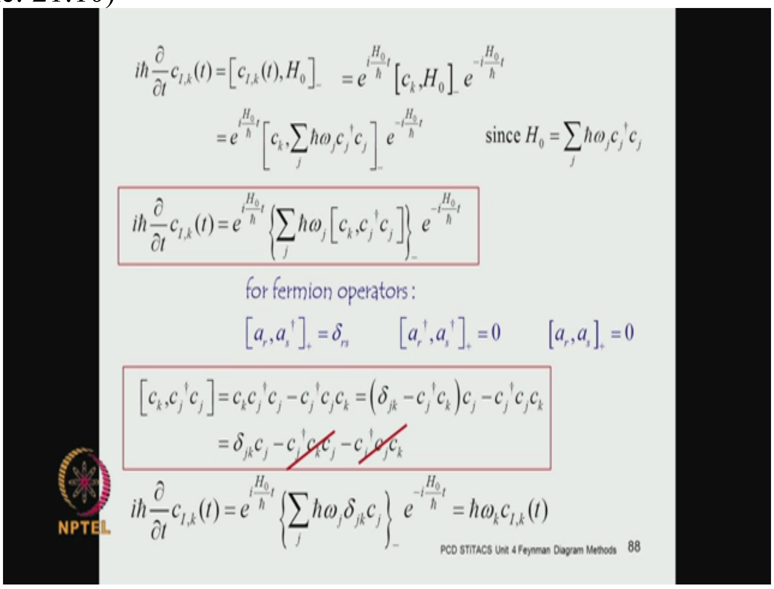

So, this is now H0 which is written in terms of the creation and destruction operators. And you can of course factor out this sigma j h cross omega j you can take it outside this bracket and then you have to find the commutator of ck with cj dagger cj and that can be determined very simply by using the fundamental commutation relations for the fermion creation and destruction operators.

So, we know what they are these are the fermion operators for and they satisfy these commutation rules rather these are the anti commutation rules okay. And using these are anti commutation rules you can work out all of these with this particular commutator of ck with cj dagger cj and you will find that it really gives you a very simple term because these two terms cancel and you get only one operator cj and that too with a nice Kronicker delta.

So, that when you carry out the summations you will be able to contract the summation and you will be left at only one term okay, so this is a very straightforward kind of analysis and you can work out all the intermediate steps one by one the PDF of all of these slides is available on the course web page. So, you can access that if you wish and now we know that you can plug in this delta jk cj over here.

And then sum over j, so with this Kronicker delta, delta jk only the term in j = k survives and this is the solution that you get now. So, the time derivative of c is proportional to c, so that has got a very simple solution. So, whenever you have any physical quantity whose time derivative is proportional to the actual amount of that quantity.

The solution involves an exponential function right. So, that is the solution that you expect and that is precisely what you get.

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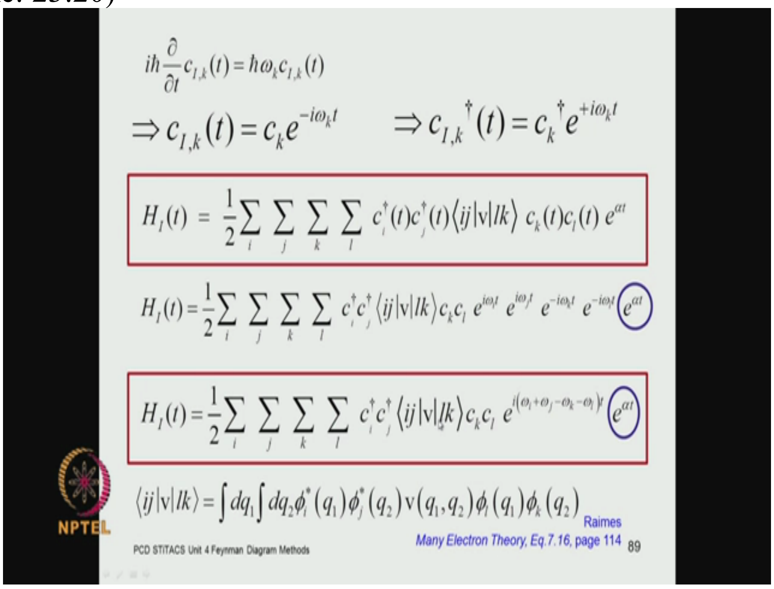

So, the destruction operator at time t is then related to the destruction operator in the Schrodinger picture and it is given by this exponential law okay. As one would expect in any similar situation you can take the adjoint of this equation and the result gives you how the creation operator behaves in the interaction picture.

So, now you have got the creation operator in the interaction picture, the explicit form of that you also have the explicit form for the destruction operator and you can use that in your interaction picture Hamiltonian corresponding to the two electron terms. Here you have the ci dagger t the cj dagger t and all of these will have these right-hand sides will give their explicit forms okay.

Likewise ck and cl t will be given by expressions of this kind okay. So, just carry over the indices carefully and now you get instead of ci dagger t you get ci dagger but then you have this e to the + i omega it which is here okay. Likewise for the cj dagger t you have got the cj dagger here and then you have got the e to the + i omega jt and from these two operators you have got these exponential functions.

But then the exponent comes with a minus sign here because these are from the destruction operators. So, there are number of time dependent terms, this is one, this is the second, this is the third and this is the fourth and these four come respectively from the for creation and destruction operators and then there is an additional time dependent term which is e to the alpha t which is coming from our adiabatic hypothesis.

That is the adiabatic switch that we have inserted as a mathematical device right. So, there are these five terms which involve time and here you just have the two center integrals which you have sufficient experience with not only from the previous units but also from earlier courses like in the Hartree Fock you deal with these two center integrals all the time right. So, these are the two center integrals and now everything over here is known.

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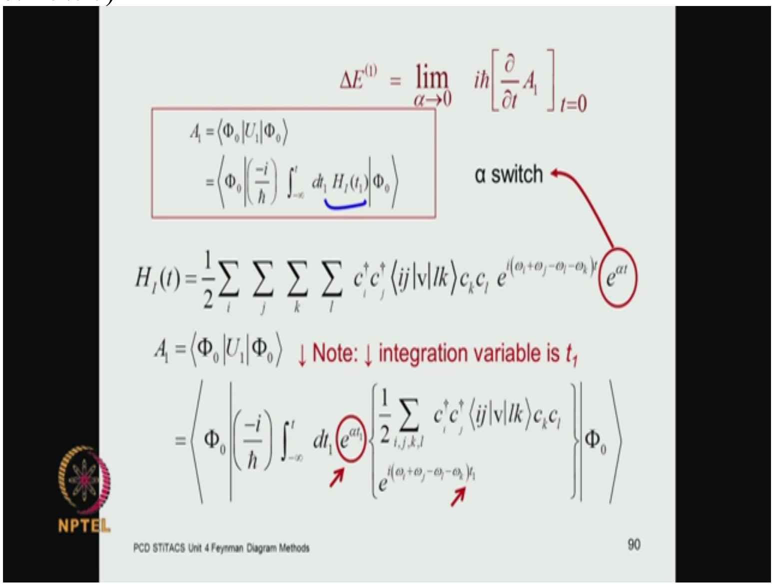

So, let us work with this and our interest is of course in determining the first order correction which is given by the time derivative of A1 at t =0. So, here you have the first order correction and you have this integral remember that time the integration variable which is the dummy variable is t1 the limits are minus infinity to the upper limit which is t which is not a dummy right not here.

So, Hi t for this particular value of t is given by these operators. The e to the alpha t has come from the adiabatic switch. So, this is the explicit form of A1 which is this and here I have plugged in this HI t1 from this equation here and that appears over here along with these four time functions, exponential functions.

And along with this adiabatic term coming from e to the alpha t, so everything has been carried forward. And the integration variable is t1 over here which is the integration variable but the upper limit of the integration over here is t okay.

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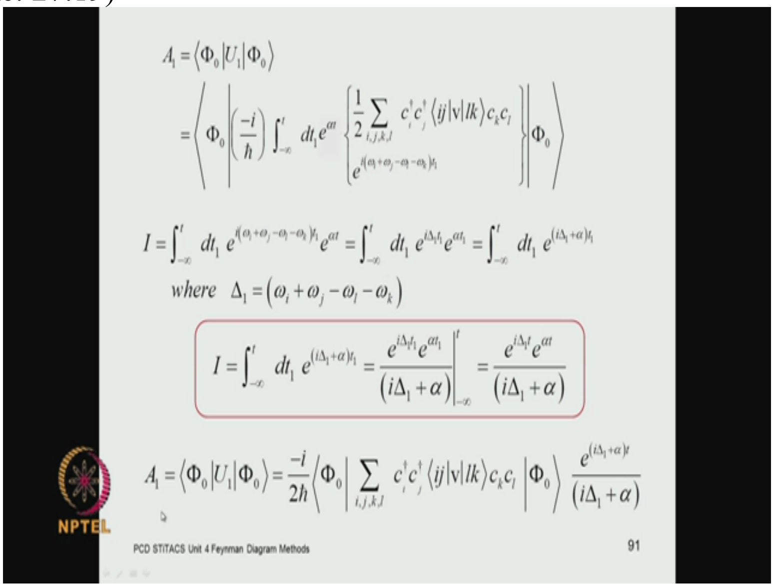

So, here of course you have got the space integrals and time integrals, so the integration over time can be carried out separately. So, I factor out this integration over all the functions which involves time and these are over here this is this e to the power i omega i + omega j - omega l - omega k t1 which is here and then e to the alpha t.

So, that function is here and this sum and difference of these four omegas is what I write as delta one okay. Again just for the sake of brevity, so that I do not have to write all those four symbols every time I work with this term. So, these four terms which include the sum and difference of these omegas in this particular with appropriate indices?

So this is what I write as delta 1 and this time integral now is just integral from minus infinity to t of this e to the i delta 1 + alpha t1. Now this is a very simple integration okay. So, what is the result you can carry out this integration and you find that after integrating it is a definite integral from minus infinity to t.

So, put the limits and this is the result that you get okay. What is also interesting is that you will subsequently be required to take the time derivative of this term with respect to time at t = 0 okay. So, that will also come out in a very neat form, so this is your result now. All the integration over the time has now been carried out and this is the result that you get for A1.

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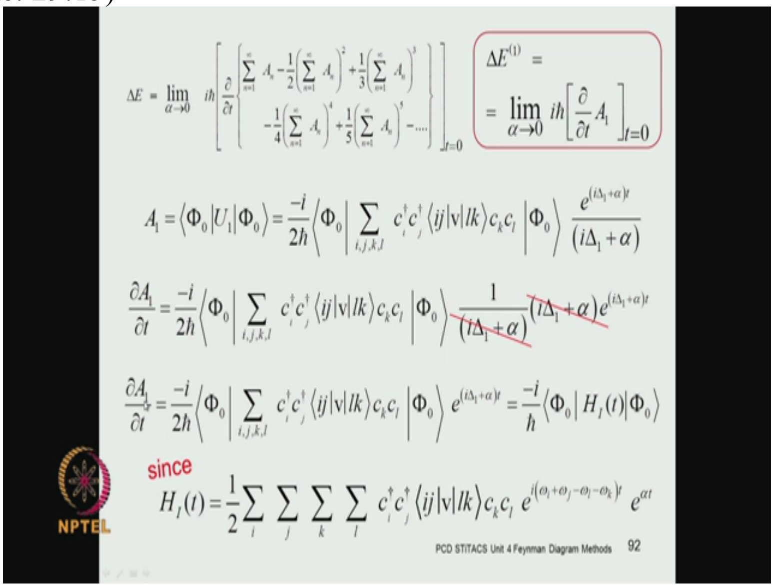

So, let us bring it to the top of the next slide and here this is our general expression for the energy correction. The corresponding correction in the first order is this and you are not interested in just A1. But in its time derivative at a particular time which is at t = 0 okay. So, this is A1 as we got on the previous slide and if you take the time derivative of this with partial derivative with respect to time.

So, this is the only term whose time derivative has to be taken what will it give you it will give you i delta 1 + alpha times this term right. So, this i delta 1 + alpha and this i delta 1 + alpha in the denominator these two terms will cancel each other you are left with only this term right. And what actually happens is that the partial derivative then turns out to be very simple over here. You just get the factor HI t over here.

So, this is what you have over here plus together with this okay is nothing but the interaction picture term for the two electron terms okay. So, this together with all those four exponential factors which are sitting over here in the delta 1 okay together with this alpha gives you essentially the interaction picture HI t. So, that is the term that you get and we will work with this term.

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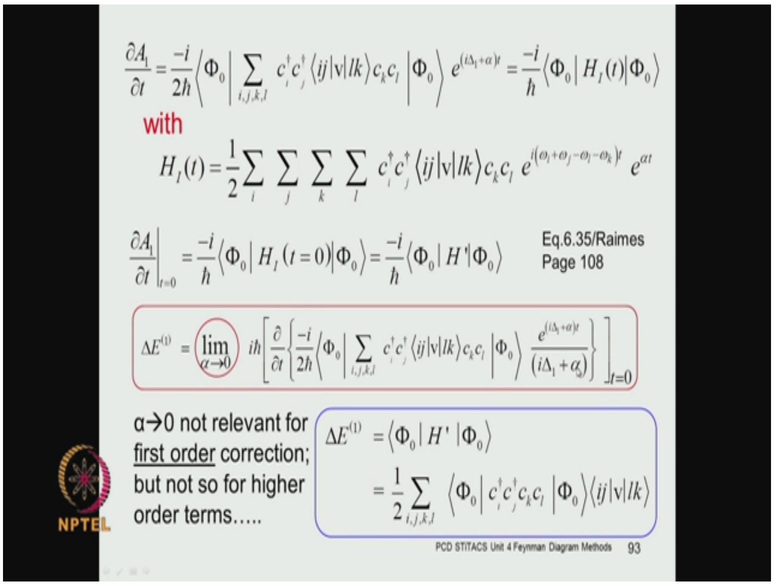

So HI t is this and now you have to take the time derivative at t = 0, so what happens at t = 0, at time t = 0 you take the time derivative of this term at t = 0 and essentially you find that alpha really does not matter okay when you take the time derivative with derivative with respect to time.

Then alpha really does not matter and in the first order correction the mathematical artificial device that you had inserted alpha really does not matter. But that is not the case when you work with higher order terms and in higher order terms you do have to keep track of these terms very carefully.

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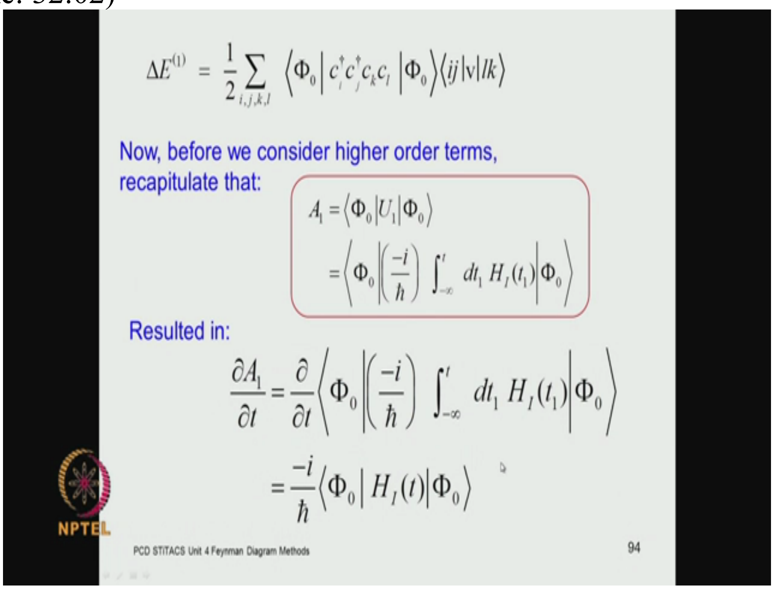

So, let us begin to look at higher order terms but before we do that let me just quickly remind you that when you express A1 as the matrix element of this time evolution operator with subscript 1, so there is only one integration involved only one time parameter involved. The result is the matrix element of the interaction picture Hamiltonian right.

This is what you get and this is a result that we will make use of when we deal with second and higher order terms. So, I just want you to remember this result at the back of your mind. So, your result then becomes independent of t1 which gets integrated out and the result does carry the interaction term Hamiltonian with the argument t okay, so that is the one that will show up in subsequent terms.

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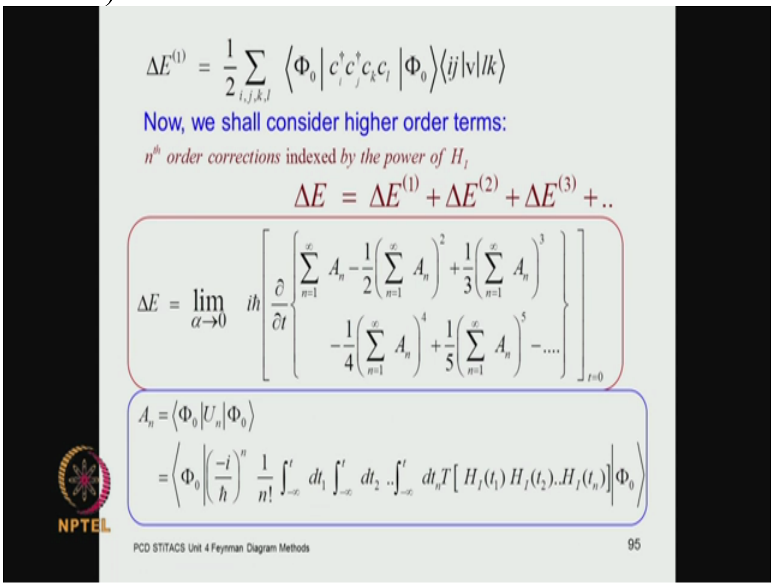

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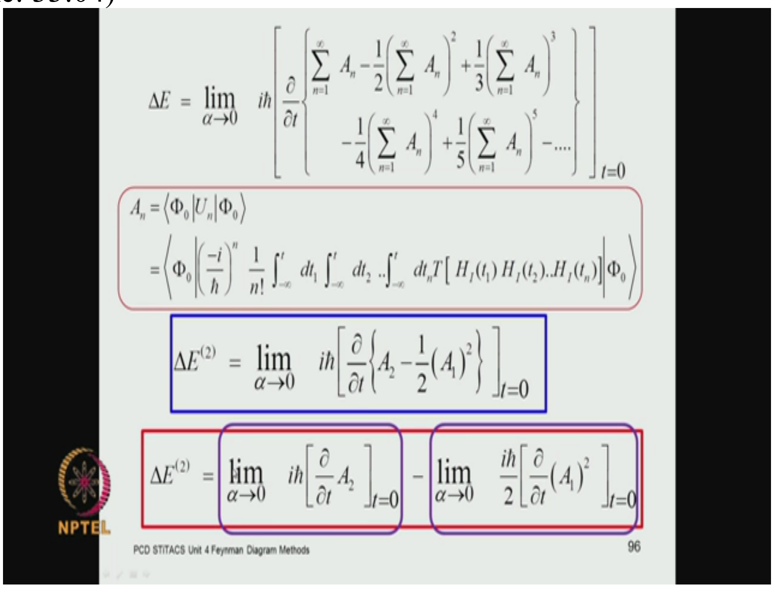

So, let us now consider higher order terms and these are the higher order terms they have got a fairly complex structure we have considered them earlier okay. So, out of these very many higher order terms now like what we did earlier that to begin with we considered only the first order term, let us now work only with the second order term. What will the second order term have?

So, the second order term will have an A2 from here and it will have an A1 square from here okay. So, the second order correction will be given by limit alpha going to 0 which is here ih cross the partial derivative at t going to 0 at t =0, partial derivative of what A2 from here and half A1 square from here okay. So, that is the second order correction that you now have to determine.

And there are two terms of for which you have to take the partial derivative. So, I will separate these now. So, I have got the partial derivative of A2 here and the partial derivative of half A1 square over here. So, I have got this ih cross over 2 and then the partial derivative of A1 square coming from the second term. So, I will now work with this the second order correction and to do that I now have to work with two terms.

One is this and the other is this, so these are the two terms that we will now work with okay and we will take them up one at a time okay. So, when you have a complicated problem what do you do you break it into pieces and then solve it bit by bit very patiently till you have solved all the pieces and then put everything together the way you do in a jigsaw puzzle okay. So, that is what we are doing over here.

So, we now are going to work with only the first term which is in this box which is the limit alpha going to 0 of ih cross times the time derivative at t = 0 of the operator A2 of the matrix element A2 which is the matrix element of U2 okay.
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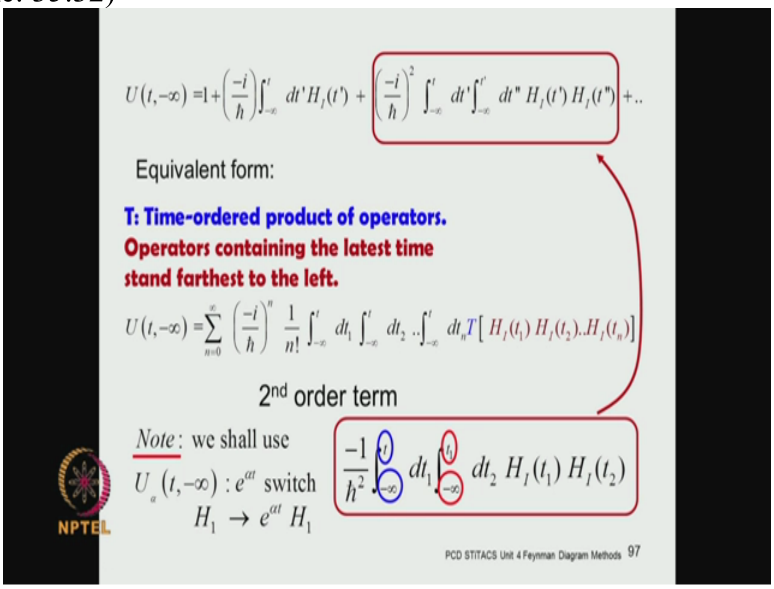

So, now we have these time evolution operators in equivalent forms okay one is an infinite series of this kind, one is an infinite series which is a summation over infinite terms each term being given as a time ordered term of a finite number of terms here. But then n goes all the way from 0 to infinity. So, these are the two equivalent forms we have demonstrated the equivalence of this discuss it in one of our earlier classes.

So, the second order term is what you get over here and instead of the variables t prime and t double prime I am going to use t1 and t2 okay. The limits are from minus infinity to t prime over here, so this is minus infinity to t1 and this limit which was minus infinity to t prime is minus infinity to t.

So, this is the second order term that we will now examine. And of course we have to keep track of the e to the alpha t. But e alpha t will come with a alpha t1 and e alpha t2 okay.
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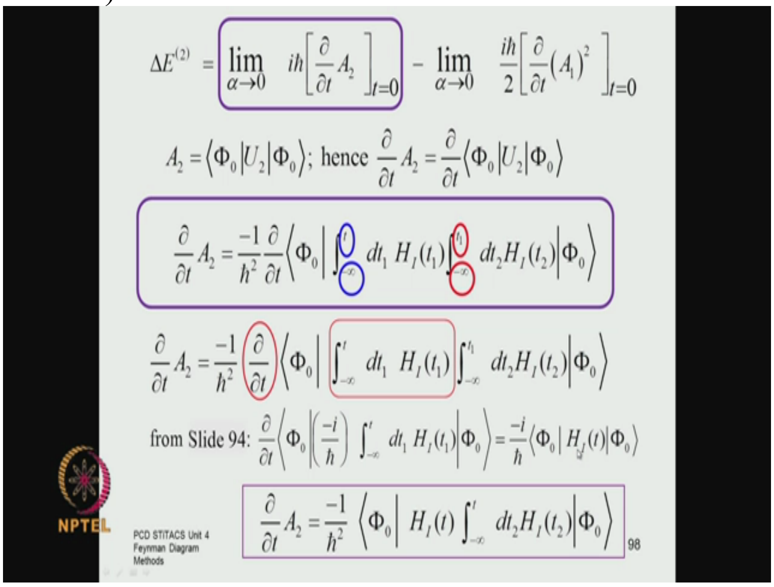

So, let us work with these two terms, so the first term is what we are now working with. So, this is what we have got all right these are the integration limits right, so I have removed these circles here just so that you can see this expression clearly. Because I want to put two other circles over here one is this del over del t over here is what I want to highlight to draw your attention to.

And then this integral from minus infinity to t which is this of dt 1 HI t1. So, this is the one I am now discussing. So, what is in this red box is what I am examined. What I am going to examine now and that is the reason I have rewritten this equation in the middle again over here is the same equation but I am highlighting different aspects of that equation as you can see okay.

And the reason to do it is because we have already determined this in our previous term for A1 okay. Because in our earlier analysis which is there in just a few slides back we already have this result that when you take the time derivative of this matrix element of the first order term, it gives you a result that you have to end up getting the matrix element of the interaction picture operator with the argument t.

Which is the upper limit of integration here okay, the dummy variable t1 gets integrated up. So, this result we have already seen and we can plug it in over here. So, we do not have to redo the whole thing, so that gives us that simple result that the partial derivative of A2 which is this left-hand side.

Is now given by the matrix element in Phi 0 and you have from this derivative and everything that is there in this red box you get the HI t okay. Which comes over here and then you have got this second integral which is from minus infinity to t dt2 of HI t2 okay.

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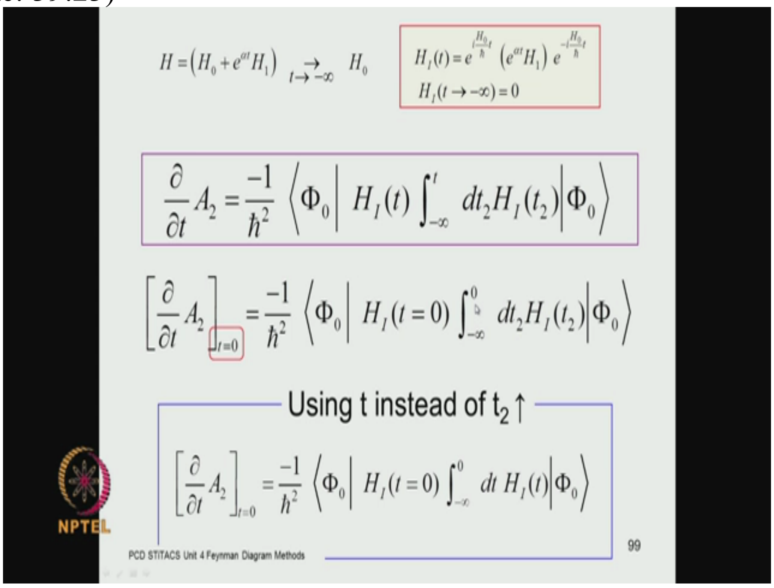

So, now this is the term that we now have to examine. (Question time: 39:29- not audible) no it is just the integration over the time, so yeah I understand what you are saying, you have got a space integral and you have got time integrals. So, the time integrals can be evaluated separately but that is the result we are using;

The same thing in the previous one if you go back now let me go take you back to the slide 95 and remind you of how we got the result here okay. This comes from the consideration of the time derivative of the time integral okay. That is all there is to it the space integral is determined completely separately. So, all the terms corresponding to the space integration all the operators they hold on to their respective places.

And the time integration over t1 is what gives you a HI t, so it is this result that we have used over here in this result over here. So, HI t and then the remaining time integration is still here but I am keeping this HI t2 to the right of this operator here. So, the time t comes as the upper limit of this integration and it comes as an argument over here. So, this is what we now have to determine.

And of course we are interested in the derivative at the particular value of t which is t = 0 okay. That is something that you should remind yourself off which means that this upper limit which is t is now 0 over here okay. Because this integration is from minus infinity to t, so this value of t has to be 0.

So, this argument of HI has to be 0 and this upper limit t has to be 0. So, this integral over t2 is carried from minus infinity to 0. And now I make a simple substitution because now I do not have t1 and t2 two time intervals to worry about so I drop the subscript 2 on t and I use t instead of t2. So, I have got the same expression but now there is only one t over here okay.
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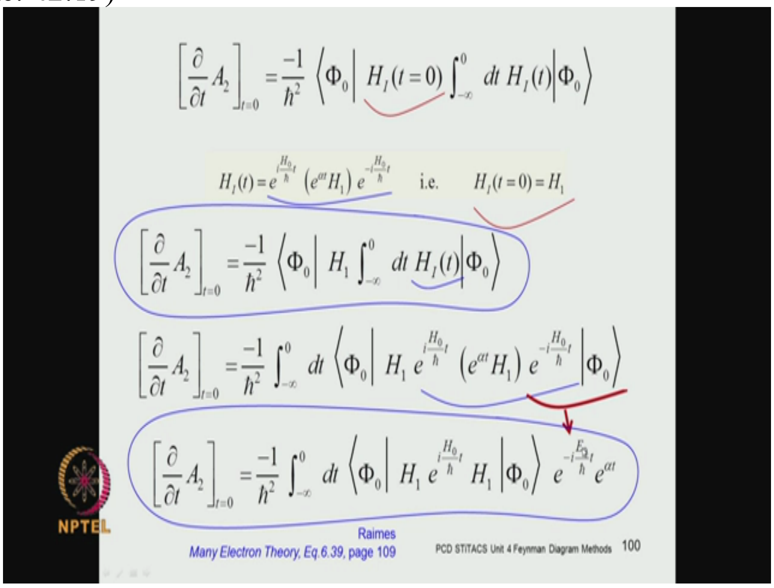

So, this is what we have to determine now what is this HI t at t =0, this is the general expression for HI t at t = 0, this factor will give you unity this factor will give you unity e to the alpha t will give you unity. And HI t = 0 is nothing but the two electron interaction term okay. So, you have that, so this HI at t =0 is nothing. But H1 now over here in the second time integral this is from minus infinity to 0 of HI t again okay.

Now here you have got a similar expression here but this is now a dummy label which is integrated out this is not the t = 0 okay. So, always remember which is a dummy label; a label is a dummy label in a particular context okay. So now key is the dummy label and it gets integrated out it is the integration variable from minus infinity to plus infinity. So, this is what the interaction term Hamiltonian is.

And this is the integration from minus infinity to 0 of dt and you can carry out a very simple analysis over here because now you know that this Phi 0 is actually an Eigen value of H0 belonging to the Eigen value E0 okay. So, you can replace this operator by the scalar E0 okay. And on this side you have to be careful because you have H1 here and not H0.

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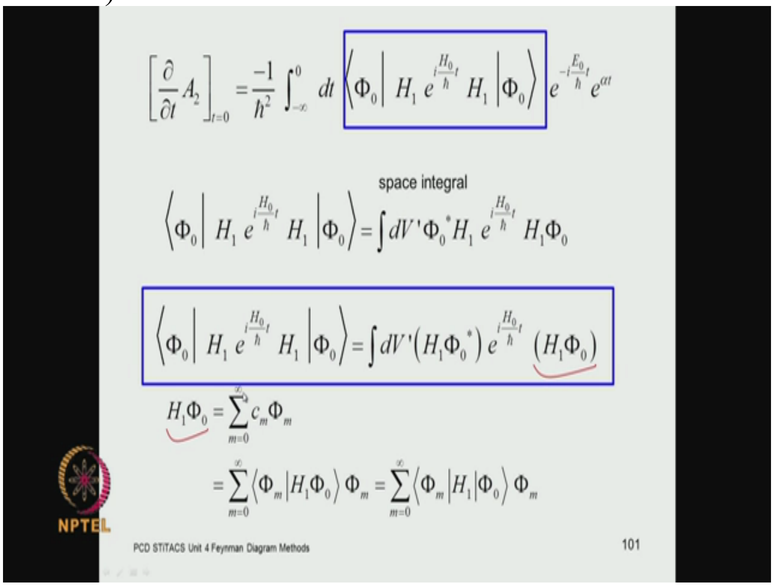

So, here the e to the minus E0 is now a scalar it is not going to operate on anything, so it just factors out as a constant. The remaining operators whose matrix elements must be determined are these okay. Now you have got a space integral this is actually a space integral right and what is the space integral this is H1 is operating on Phi 0 star okay. This is the hermitian operator, so it can operate to the left.

So, you have got H1 operating on Phi 0 star and H1 when it operates on Phi 0, Phi 0 is not an Eigen value of H1. So, the result can nevertheless be expressed as a linear superposition of all the unperturbed states. And all the unperturbed states are the Phi m's with Phi m going from 0 to infinity.

So, this is a complete basis and these are normalized functions okay normalize base functions and the coefficients cm are nothing but the projection of this on a particular mth base element right. So, these are the coefficients which are the matrix elements of the operator H1 which is the interaction of the operator between two unperturbed states. So, this is the expansion of H1 Phi 0 and you can plug in this expansion over here.

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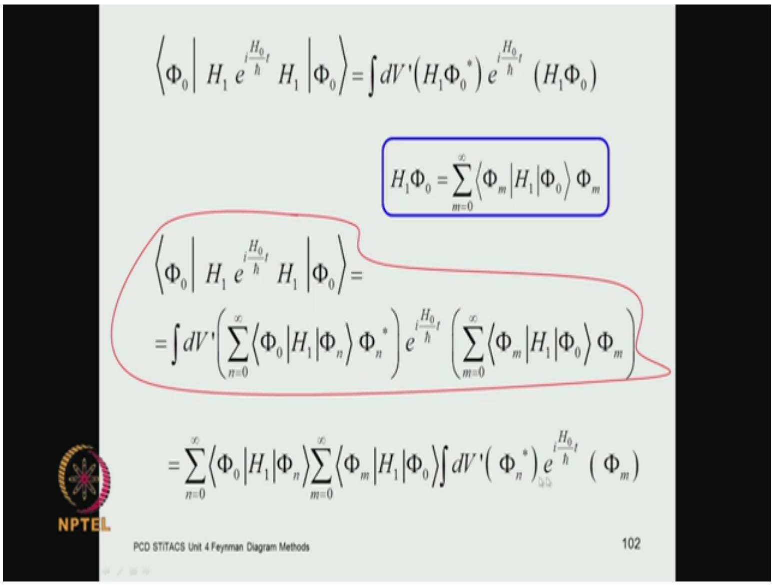

So, let us do that so this is an infinite expansion. So this infinite expansion from m = 0 to infinity comes here. You have got H1 Phi 0 over here and H1 Phi 0 on the left. So, one of them gives you a summation over n with the complex conjugate over here. The other gives you a summation over m which is without the complex conjugate okay.

So, there are two summation indices one is m and the other is n. And now your space integral over here takes a rather simple form because both of these are Eigen values of H0 okay.

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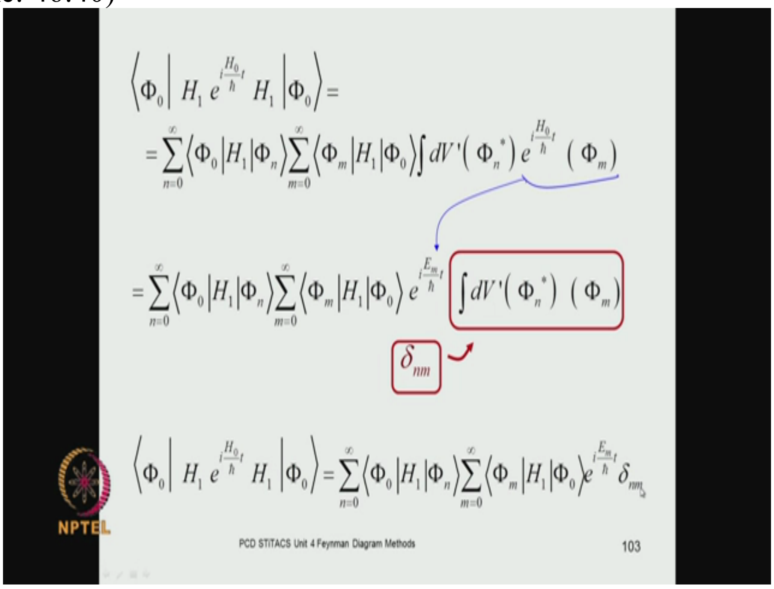

So, both of these being Eigen values of H0 you get the e to the i E mt because Phi m is an Eigen value of H0 belonging to the Eigen value Em. So, you get e to the im over h cross t this you can always factor out okay. And then you have a space integral of Phi m star with Phi m which is nothing but the ortho normality integral.

So, if n = m you will get 1 and if n is not equal to M you will get 0. So, you have got the orthogonality over there that gives you the Kronecker delta, delta nm. And then you can sum over one of these either m or n and then contract that so you are now left with this after you sum over this m with delta nm.

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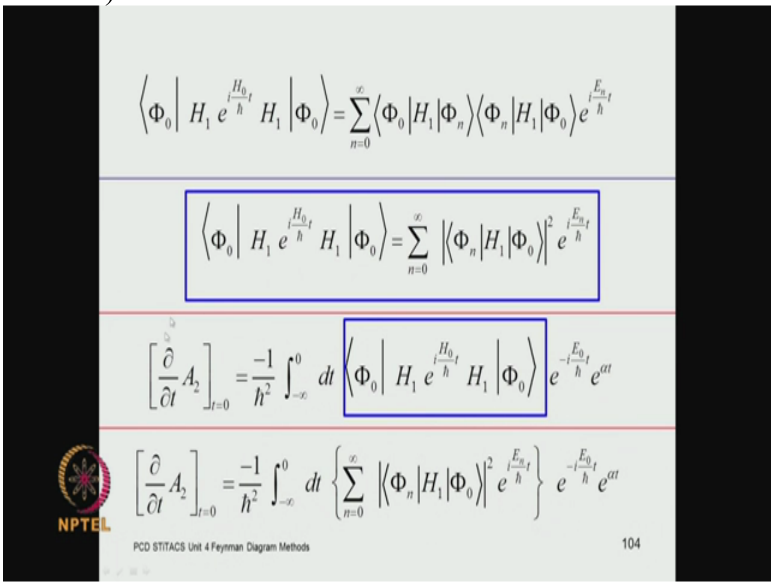

You are left with only one sum which is sum over n going from 0 through infinity and you have these two matrix elements and you have got a scalar here right. Now what are these two terms these are just complex conjugates of each other. So, you take the modulus square okay. So, now the whole expression is being simplified to a substantial extent not enough but much better than what we started out with okay.

Now you will have to take the limit of the derivative at t = 0, so this matrix element which is here can be substituted by what you have on the right-hand side okay. Let us do that so whatever was here on the right hand side comes here in this beautiful bracket okay. You are following all the terms okay.

This very simple substitution it takes a lot of time to write this because every time you write it you make a number of careless mistakes. You write t2 in place of t1 and then you are out for a toss okay but do it carefully you will get it right. So, over here in the class I just want you to concentrate on the logic on how things are done okay.

And then you can work it out yourself if you need any reference the PDF files of these slides are of course available on the course web page. So, here you now take this expression, so this is the results from the right-hand side which is borrowed here in this beautiful bracket.

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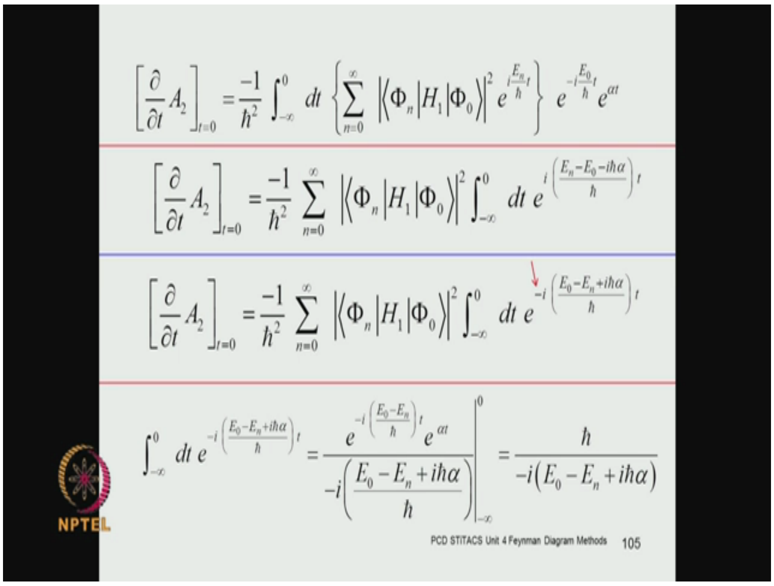

So, let us write it here at the top and what do you get over here. So, you separate this space integral from the time integral, so you have got the time integral from minus infinity to 0 but what is time dependent over here this piece is not time dependent it is this piece which is time dependent. And this piece which is time dependent and this piece which is time dependent.

So, you carry out the integration over the time variables separately over here and again you have got a very simple time integral just as you had in the earlier cases it is just the time integral of an exponential function everybody knows how to do it okay. So, now evaluate that time integral put the limits minus infinity to 0 this is the result that you get okay. That is high school integration all right.

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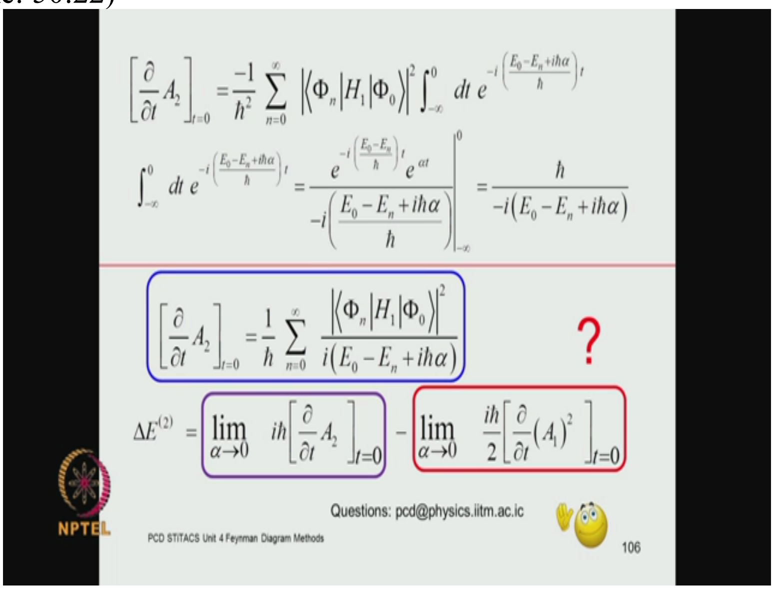

So, let us use this result so this is the result of the time integration and we now get the partial derivative with respect to time at of the element A2 at t =0 which is given by this term at t = 0 this is what it turns out to be. So, you have got this you are you have to take care of the powers of h cross say what 1 over h cross squared over here, you have got h cross over here, so you end up with 1 over h cross.

You have a -1 sign there is a minus sign over here okay, so that takes care of it. So, you have to keep track of all these details do it carefully you will get it right. Raimes write these results in natural units in which he puts h cross =1 and then you do not see h cross and then it is very easy to make a mistake of the powers of h cross which is why I have done this analysis inclusive of the factor of h cross.

So, that you carry it carefully when you do calculations of course you have to plug it in okay. So, this is the result pertaining to this box over here right. So, these are the two terms that we wanted to determine. We have succeeded in getting the first box it has taken as a full class to do this. So, we postponed the determination of the second term for the next class okay.

Questions too many terms too many complexities but everything finally comes down to somewhat simple terms and the beauty of this whole analysis is that instead of writing a large number of terms time derivatives integrals and so on. We will then be able to express the importance of these terms using some very nice cartoons.

So, those are the Feynman diagram that you are looking for and that is what this unit is about we have already had four classes in this unit and you have not seen those very nice pictures yet but they are coming. But it needs a lot of background to do that, so we already had four hours of background. Now let us see when we get to that eventually we will that is what this unit is about okay.