Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'

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Lecture 27
Gell-Mann and Low Theorem

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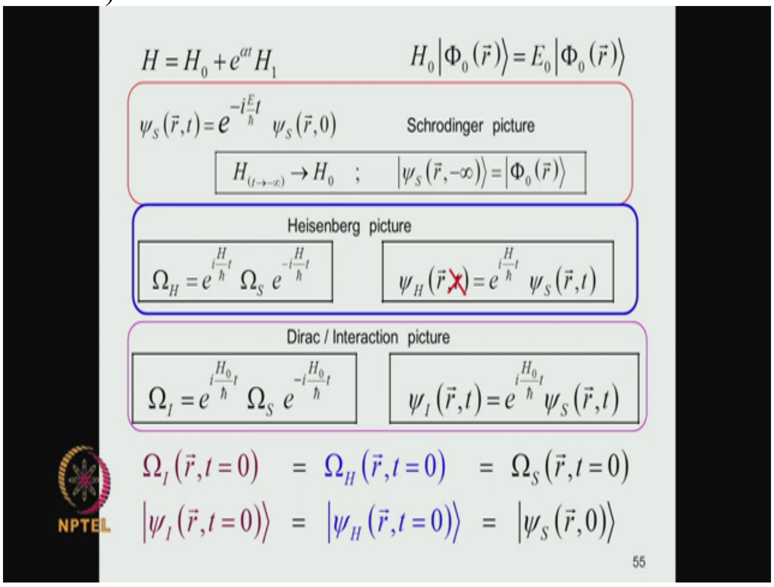

Greetings, will discuss the Gall-Mann and Low theorem which I mentioned in the previous class and essentially let me quickly remind you what we are really dealing with because our focus is on the treatment of the electron correlations which we are very concerned about. We know that the Hartree Fock is not able to deal with these electron correlations.

The Hartree Fock certainly took account of the statistical exchange correlations but not the Coulomb correlations. So, we introduced quantum mechanics in various pictures the Schrodinger picture is the one that we most often use in undergraduate and you know some of the introductory graduate level courses.

But then there are other pictures which are very useful in doing quantum theory of many particle systems in particular the Heisenberg and the Dirac pictures. So, this is what we have in the Schrodinger picture and then what we did is to introduce the difficult term this is what I have been calling as the unfriendly term. This is what makes the problem so cumbersome the H1 and you have the exact solution for H0 which is the unperturbed Hamiltonian.

So, this is solvable this solution is known we have the solution with us. But then we do not have the solution when we include the correlations and these are sitting in this term H1. So, what we did was to insert a mathematical parameter. Now this is the control parameter that is at the disposal of mathematicians.

And it is not that there is anything in nature which lets us choose the presence or absence of correlations. But the physicist uses his tools, mathematical tools and we can choose up properly values of alpha or t which are useful to us so that we can develop a methodology which can be exploited to get the solution for the full Hamiltonian which of course is H0 + H1.

The full Hamiltonian is H0 + H1; H1 is the difficult part of the Hamiltonian the unfriendly part of the Hamiltonian which makes it impossible to use a perturbative treatment. Like in the many electron system the first order perturbation theory gives you the same result as the Hartree Fock. But second order perturbation theory and higher order perturbation theory does not converge.

So, this is the unfriendly part and we sort of scale this unfriendly part by this term e to the alpha t and the choice of the parameter alpha when alpha = 0, you have e to the power 0 which is 1 and you have got the full Hamiltonian. When t = 0 which is the instant of time you can say that it is the now moment for us. This is when we really want to deal with the full Hamiltonian.

So, at t = 0 again you have the full Hamiltonian but then if you look at the system evolution from t = or t going to minus infinity like this is the position vector r and this is the time which goes to minus infinity then as t goes to minus infinity this e to the alpha T times H1 goes to 0 and you have only the unperturbed Hamiltonian.

And that is the part of the problem for which we do have a solution and our effort is going to be always from the known to the unknown and what we do know is the solution to the H0 and we have to figure out what is the solution to the full Hamiltonian which is H. So, in the Heisenberg picture we carry out these transformations. So, these are the transformation of the operators and this is how the Heisenberg state transforms.

You get it from the Schrodinger picture wave function and the Heisenberg picture wave function of course does not depend on t. All the time dependence is packed in the operators the state functions themselves are independent of time in the Heisenberg picture. In the Dirac picture which is also called as the interaction picture at times. Here the transformation is again through a unitary operator.

But whereas the unitary operator over here was the full Hamiltonian, in the Dirac picture it is only the unperturbed Hamiltonian okay. So, it is not the same but it is similar but not the same here the transformation is through the unperturbed Hamiltonian and the wave functions also transform like this.

And the result of this is that both the wave functions and the operators in the Dirac picture depend on time. So, at t = 0 which is the now movement as I call it. So, at t = 0 all the operators correspond exactly equal to each other and so do the wave functions at t = 0 okay. They all correspond to each other at this now moment. But otherwise that all other instants of time they are different.

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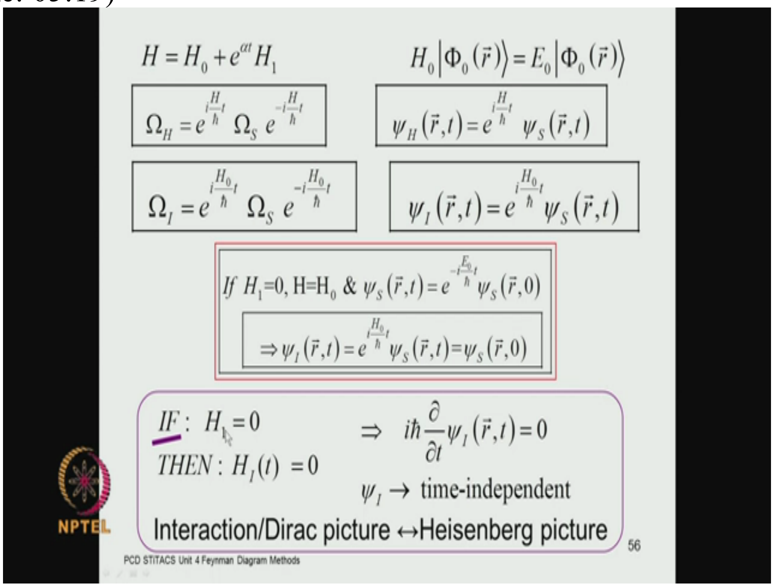

So, these are the primary relations that we work with and here notice that if this unfriendly part was simply not there okay. If the H one was 0, if the correlation part was 0 just in case wishful thinking, if it was 0, if H1 was 0 then H would be H0 right. And this is how the Schrodinger picture wave function would evolve with time from time t = 0.

And the interaction picture wave function would be the same as the Schrodinger picture wave function at t =0 okay. So, that is a particular case and what it really does is that just in case H1 were 0 which we know it is not but in case if it were 0 then this wave function would become independent of time in the interaction picture.

So, these are some special cases in which the Heisenberg picture and the interaction picture or the Dirac picture they correspond to each other but so these are special situations.

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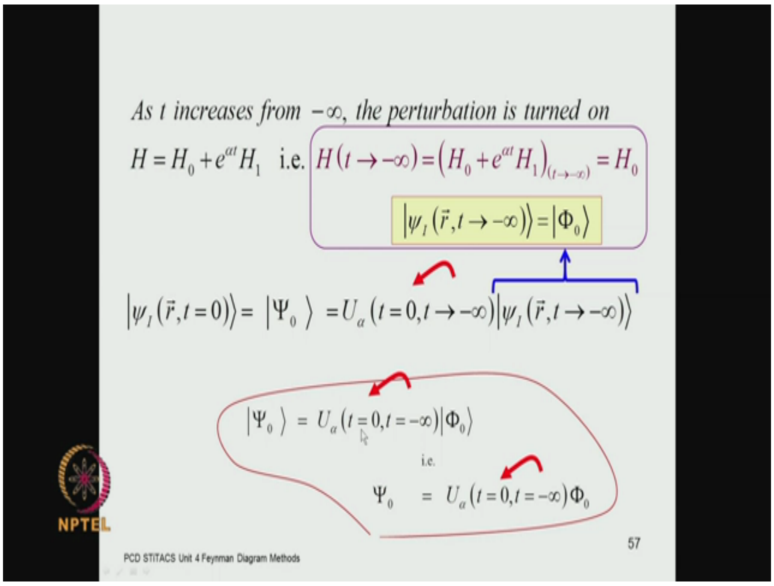

Now what happens when you go to minus infinity as t goes to minus infinity the Hamiltonian which is the full Hamiltonian this t going to minus infinity kills any effect of this H1 in this product term. And then you have only the unperturbed Hamiltonian and the wave function at t equal to minus infinity.

In the interaction picture is nothing but the solution to the Schrodinger equation in the Schrodinger picture corresponding to the unperturbed Hamiltonian and that is the known thing it is this known from which we want to go to the unknown, so Phi 0 is known to us. Now the interaction picture wave function at t = 0 is what I represent by this size 0. So, this 0 subscript really corresponds to this time t = 0.

And we are looking our interest is in the interaction picture, so that is the one that we are going to be using in our analysis. So, this state can be obtained from the state as t goes to minus infinity by operating on this by the time evolution operator this is U. So, this is the unitary operator which tells you how the state would evolve from t at minus infinity and gives you the state at t = 0.

So, the unitary operator is this is the time evolution operator it actually tells you that if you know the wave function at t equal to minus infinity or t tending to minus infinity then how do you get the wave function at t = 0. So, this is the unitary time evolution operator and this one is nothing but the Eigen state of the unperturbed Hamiltonian Phi 0.

So, if you know Phi 0 and then you know this unitary operator then you can get the interaction picture state. So, that is the strategy that we are going to adopt okay. So, this is what we it really boils down to. We will get the interaction picture solution state vector at t =

0 from the Eigen state of the unperturbed Hamiltonian through the time evolution operator U by fixing these two parameters for time.

Which is t equal to minus infinity which is the start time and t = 0, which is the end time over which this evolution is observed. You can write it as vectors in the Hilbert space or a state functions, so any which way, so it is just a matter of notation.

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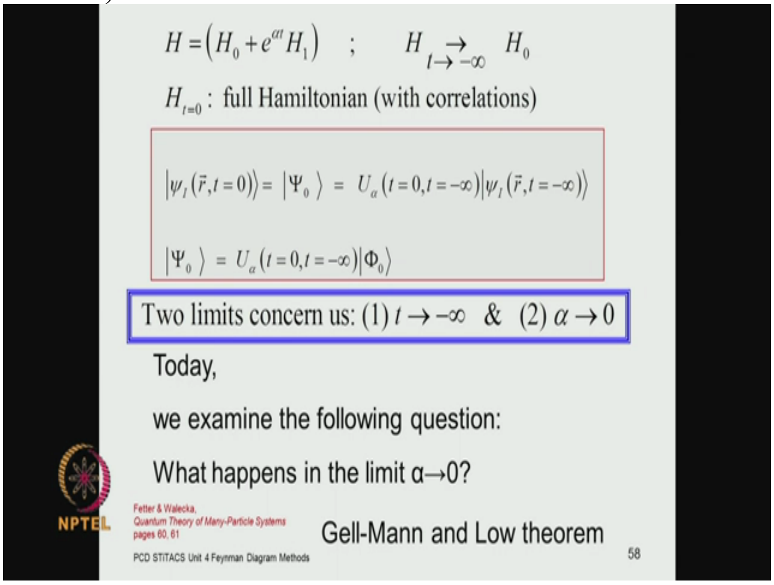

So, this is what we have got and there are these two limits which are off importance to us, as t goes to minus infinity we know that we have the unperturbed problem. The alpha tending to 0 alpha going to 0 is when you will have the full Hamiltonian that is the real problem of interest to us that is precisely the problem that we want to solve, t going to minus infinity we have discussed how we get the solutions right.

Because that is just the unperturbed part of the Schrodinger equation, so that we know how to handle and the question is what is going to happen when you take the limit alpha going to 0. And this answer to this question what happens in the limit alpha going to 0 is provided by the Gell-Mann and Low theorem of quantum theory.

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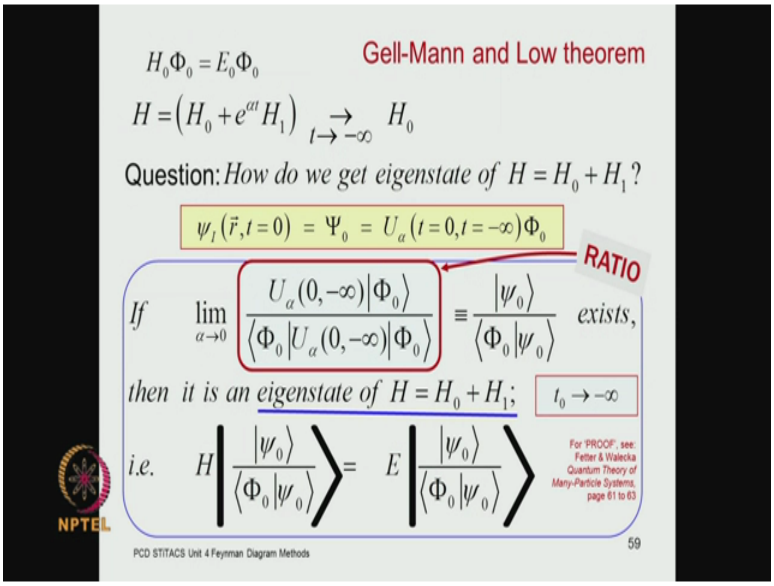

So, this is a very fascinating theorem let me state what the theorem is and you can see the entire discussion in the Fetter and Walecka's book. So, you have got the unperturbed part of the Schrodinger equation this is solvable. Then you have the full Hamiltonian which reduces to the unperturbed Hamiltonian in the limit t going to minus infinity.

And we are addressing the question how do we get the Eigen state of the full Hamiltonian from Phi 0. So, that is the question we are really interested in. Now we do know that the Eigen state in the interaction picture at t = 0 can be obtained from the unperturbed solution through the time evolution operator.

This is the one which of course has the correlation sitting in. So, that is how it is going to pick up the correlations and you will see it explicitly in the slides that follow. So, this is the statement of the theorem, the theorem states that if the limit alpha going to 0 of this ratio exists okay.

This is a limit which is written as Psi 0 over the projection of Psi 0 on Phi 0, so this is the inner product okay. So, if this limit exists then the theorem states that it is an Eigen state of the full Hamiltonian and you can write it as an Eigen value equation H operating on this state is equal to E operating on that state. You essentially get an Eigen value equation for the full Hamiltonian provided the limit of the ratio exists.

Now mind you, you are interested in the limit of the ratio and you have got U alpha in the numerator, you also have it in the denominator. You have essentially the average value of the time evolution operator in the unperturbed ground state Phi 0 that is what you have in the denominator right. And both the numerator and the denominator have the parameter alpha which is our mathematical construct.

And one could in principle ask what is the limit of the numerator in the limit alpha going to 0, one could also ask the question what is the limit of the denominator in the limit alpha are going to 0. Now it turns out and I will not have a chance to go through this in too many details, I am not going to work out the detailed proof of the Gell-Mann and Low theorem. I will refer you to just two or three pages from Fetter and Walecka's book.

The reference is provided here and it turns out that the limits of the numerator and the denominator if you take them separately you do get certain divergences and these limits do not even exist in the sense that they are not very well-defined okay. But it does not matter because if whatever factor is unknown when you see the limit for the numerator cancels the corresponding factor in the denominator exactly.

Then the limit of this ratio is very well defined and that is the one that we are really concerned with because we are not using the limits of the numerator or the limit of the denominator separately. We are interested in limit of the ratio and that is well defined and this is the sum of these things go into the details of the proof in the Gell-Mann and Low theorem.

And essentially what this theorem tells you is that if this limit is defined and this is the limit the limiting value of what is in this box is written by this ratio here. This turns out to be an Eigen state of the full Hamiltonian and this difference between E, this is the Eigen value of the full Hamiltonian E0 is the Eigen value of the unperturbed part of the Hamiltonian.

The difference between them is the correlation energy which the unperturbed problem is not able to address, so that is the one that we are trying to find out.

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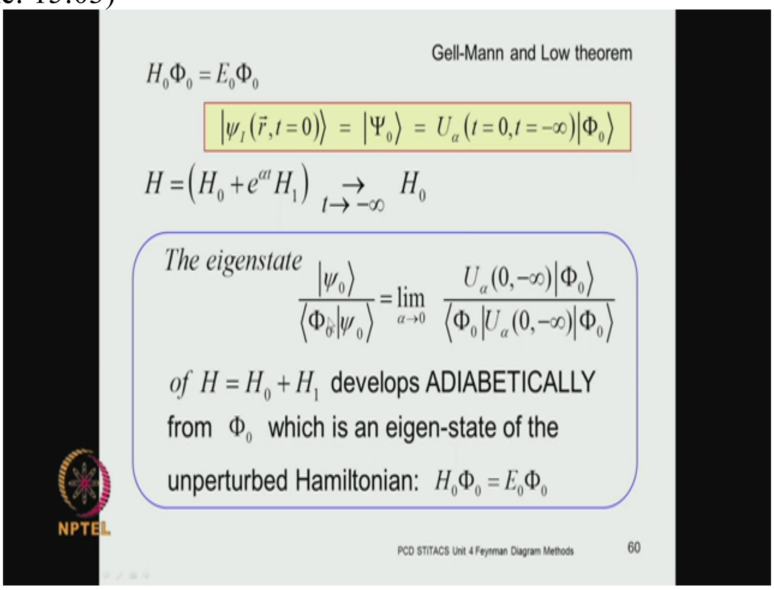

So, the contention of the theorem is that this particular Eigen state which is which we met in the right hand side of the Gell-Mann and Low theorem this is the same vector. So, this particular vector which is obtained in this limit, it gives you an Eigen state and this Eigen state develops adiabatically from the Eigen state of the unperturbed Hamiltonian.

Adiabatically in the sense that you are not adding any external field any perturbation external field and in that sense this is an adiabatic evolution of the state which is an Eigen state of the full Hamiltonian inclusive of the correlation from the solution that you have for the unperturbed Hamiltonian.

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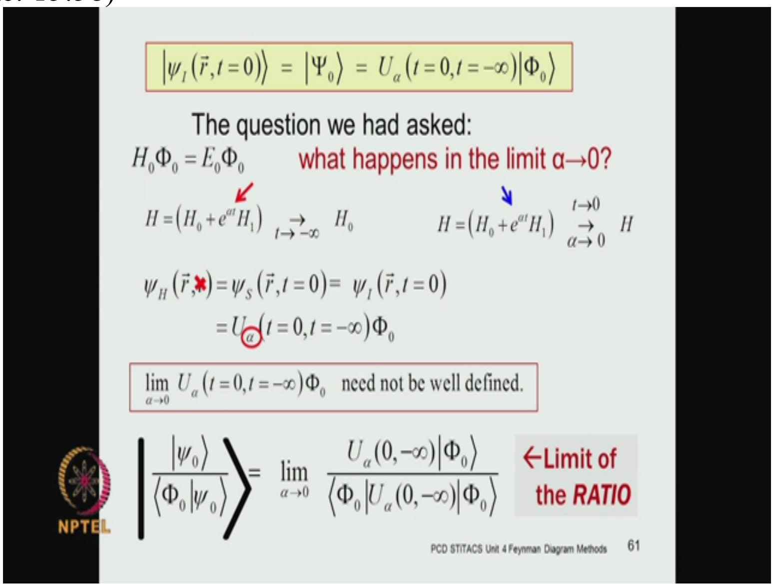

So, this is our question what happens in the limit alpha going to 0. So, we are okay with this part and we are concerned with the limit alpha going to 0. So, mind you that as alpha goes to 0, you get the full Hamiltonian. But as t goes to minus infinity you get the unperturbed Hamiltonian.

And this Hamiltonian gives you the full Hamiltonian in the limit alpha going to 0 and also as t goes to 0 which is the now moment for this problem okay. So, also in the limit t going to 0 or alpha going to 0, so our interest is in the solutions at t = 0. So, that is the instant of time in which we are interested.

So, this is how the wave functions of the different pictures are related I mentioned that this limit need not be well-defined it is not fundamental to our analysis. It is the limit of the ratio which is of importance to us. So, these are some of the things that I really want to emphasize okay.

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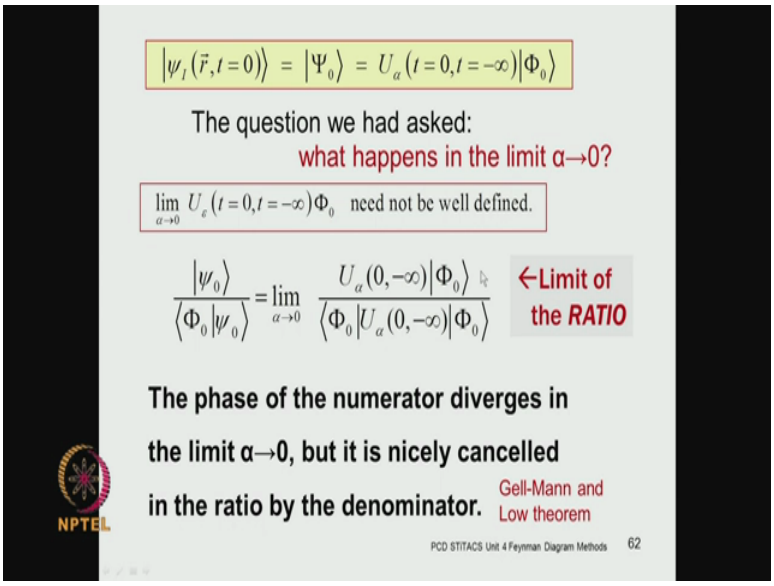

What happens is that there is a phase factor and you get certain divergence in that in the numerator. If you were to treat this separately and you would have a corresponding divergence of the denominator as well and they happily kill each other when you take the ratio.

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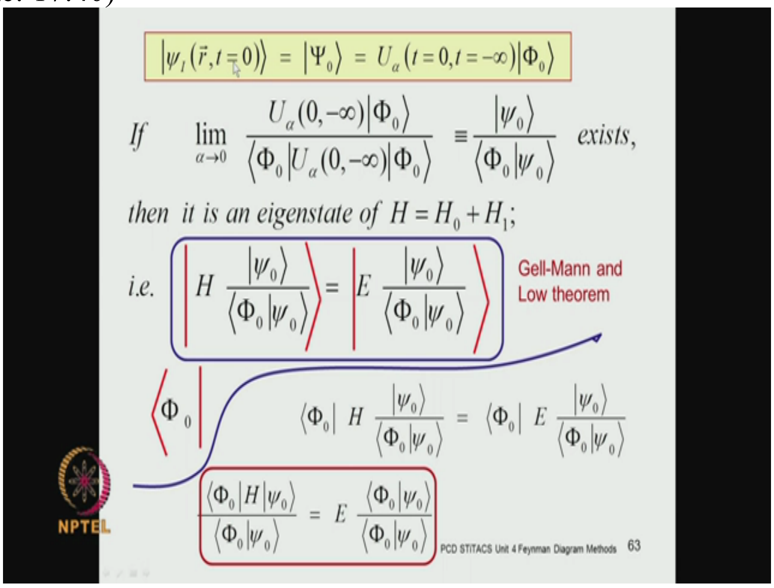

So, now let us begin with the statement of the Gell-Mann and Low theorem and what we are going to do is to look at this whole thing as a vector. Because when this operator operates on a vector you get a new vector that new vector is what I put in this larger ket which is coloured in red okay. So, now let us look at these two vectors on the left side and on the right side. You have got a ket vector.

And I am going to construct an inner product of this vector which is to take its projection on another vector which is the adjoint of the vector corresponding to the ground state of the unperturbed Hamiltonian okay. So, the unperturbed Eigen state Phi 0 is known to us. So, we have the adjoint of that vector and I take the projection of this vector which is in this larger ket the red coloured ket.

And I take the projection of this on this so it is just the inner product that I am constructing. So, let us go ahead and write this projection. So, it is it will be this, it is the projection of this vector on Phi 0 on the left hand side. On the right hand side it is the projection of the right hand side on Phi 0 okay.

Now let us write these terms a little bit neatly because in the numerator you will have the matrix element of the full Hamiltonian in the states Phi 0 and Psi 0 okay. So, let us rewrite this result a little bit neatly, so you have got the matrix element of the Hamiltonian in these states.

This is the Eigen state Psi 0 which is here this is the Eigen state in the interaction picture at t = 0. So, this is just the solution that we really want okay. So, this is what we are interested in and you have got the Hamiltonian operating on this Psi 0 and we are taking its projection on Phi 0 okay. So, this is the result that we have got.
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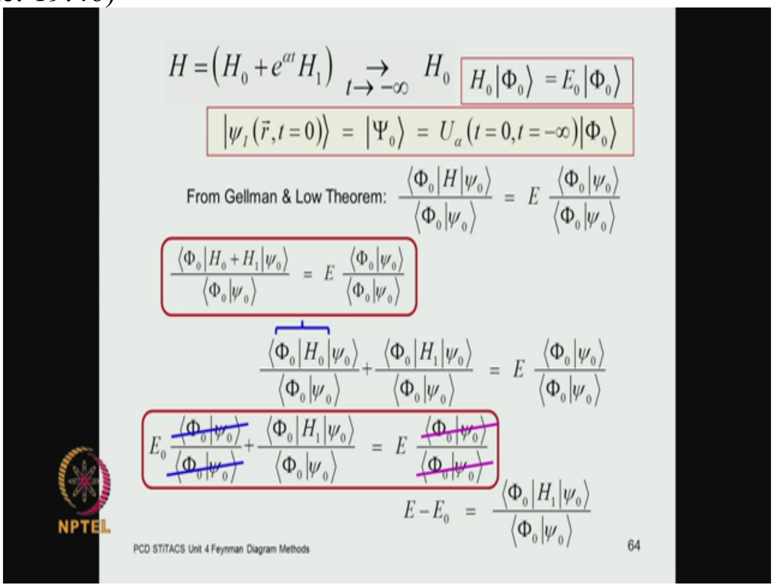

So, let us write this result over here which we got this result using the Gell-Mann and Low theorem right. We just took the project of the Gell-Mann and Low vector on the unperturbed state vector Eigen state of H0, so this is what we have got. Now this is the full Hamiltonian which has got two pieces one is H0 the other is H1. So, I am going to separate out the contributions from these two terms.

So, on the left hand side I will have two terms so you this is the first term which is the matrix element of H0 in these two states. And then in the second term you have got the matrix element of the unfriendly Hamiltonian the perturbation H1 in these two states. Now here you have an Eigen value equation because Phi 0 is an Eigen state of H0 right. So, Phi 0 H0 on the left over here will be E0 Phi 0 because it is just a Eigen value equation over here.

So, here you get E0 Eigen value pops out and then you get the projection of Psi 0 on Phi 0. Now Psi 0 and Phi 0 of course are different so the projection of Psi 0 on Phi 0 is not equal to unity okay. Both are normalized then the projection of Psi 0 and Phi 0 would be 1 if they were the same Eigen state. But they are not the same and therefore it is not unity it would be some nonzero value.

But whatever it is you have the same factor in the denominator here okay. So, these two factors cancel okay. Likewise these two factors cancel okay and now you have got the Eigen value of the full Hamiltonian on the right side. On the left side you have got the Eigen value of the unperturbed Hamiltonian plus this term.

So, if you just rearrange the terms of this equation you get the difference between the Eigen values of the full Hamiltonian and the Eigen value of the unperturbed Hamiltonian. So, E - E0 which is like the correlation energy, so you get this in terms of the ratio of these two quantities okay.

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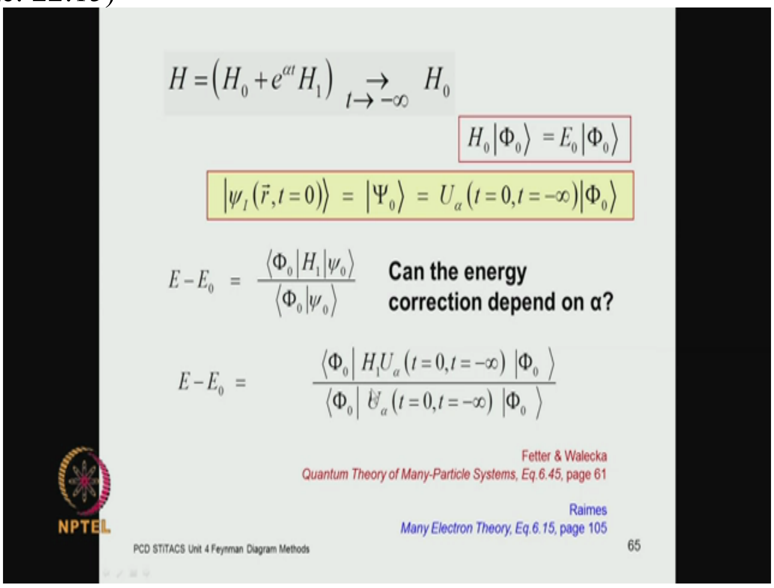

So, let us figure out how we are going to evaluate this, this is the quantity of interest to us. Now H1 okay, so the Psi 0 over here we know can be obtained from Phi 0 through the evolution operator U. By taking the evolution from the state minus infinity because this is the solution at minus infinity. This is the solution of the unperturbed Hamiltonian and that is what the full Hamiltonian collapses into as t goes to minus infinity.

So, we know this and from this you can get the solution at time = 0 through this time evolution operator as we have just discussed. So, you have this Psi 0 written over here, you do the same in the denominator this Psi 0 is also this then you have got H1 over here, so this is the result that you have got. However our result cannot really depend on alpha which is only a mathematical construct.

But that is not a worry because anyway we are taking the limit alpha tending to 0 okay. So, that is the limit that we are going to discuss. So, this is our expression this is how you can get the states. Now the state vectors which are involved which here okay. You see a Phi 0 here and a Phi 0 here, you see a Phi 0 here and a Phi 0 here.

So, all the state vectors that you need to evaluate the right hand side are now known to us. So, we have succeeded in writing the difference E - E0 in terms of state vectors and the time evolution operator and the correlation term okay. But using only those vectors which are known to us because that is the Eigen state of H0 that part of the problem has been solved.

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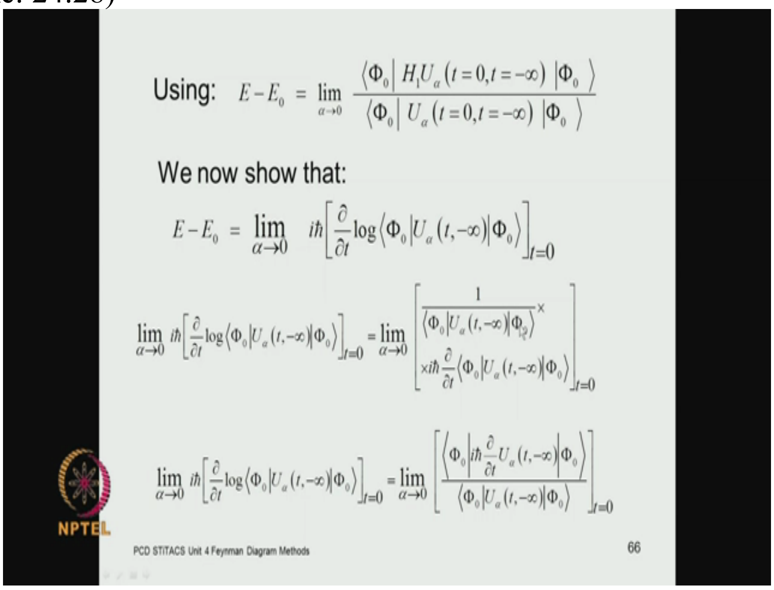

Now this is the result the one at the top we just got this from the Gell-Mann and Low theorem. Using this result we will now show that this energy difference is actually equal to the limit alpha going to 0. And here on the right hand side I have got a new expression and we are going to see how this result shows up.

It will turn out in the next few minutes that if you take the logarithm of the expectation value of the time evolution operator in the state Phi 0. Then take the limb the derivative of this log with respect to time, the partial derivative then evaluate the value of this partial derivative at t = 0 and then take the limit alpha going to 0, so go in that order. First take the log then the derivative that the value of the derivative at t =0.

And then finally will limit alpha going to 0, so do not do anything in any arbitrary order because that is the sequence in which things have to be done okay. So, let us look at this right hand side, let us look at this limit alpha going to zero of this expression on the right which is ih cross del by del t of this log at t = 0. So let us consider what is inside the square bracket this is just the time derivative of this log.

So, it will be this 1 over this expectation value times, the time derivative of this expectation value right. And I have pulled it this factor ih cross over here inside the bracket and then of course I retain the t going to 0, constraints because that is the one which is of importance. So, this is what we have got so the limit alpha going to 0, ih cross del over del t, so this the left hand side.

And now I just write this a little bit neatly. So, that I have got this factor in the numerator which is this and this fact factor in the denominator comes below it, so I have just rewritten this expression so that it is easy to read.

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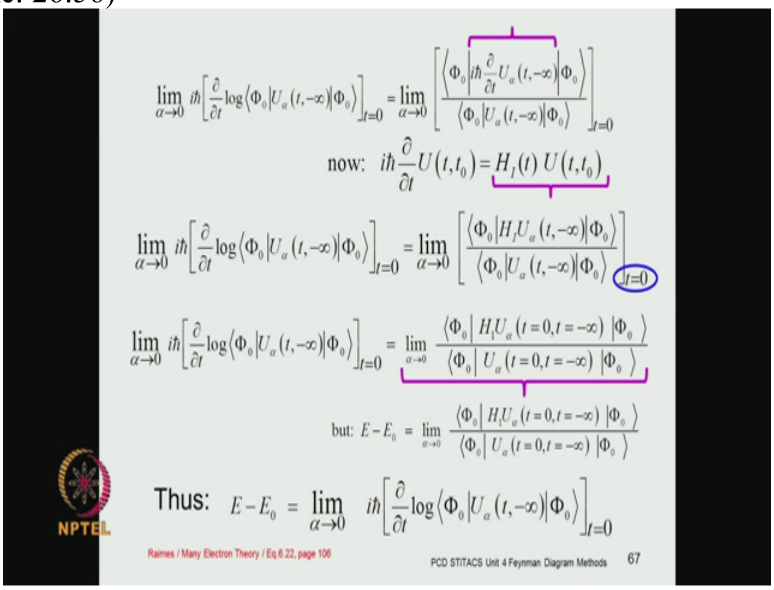

So that is what we have here at the top of this slide. Now what is this? This is nothing but the Schrodinger equation for the time evolution operator in the interaction picture right. So, in the interaction picture the time evolution operator satisfies the differential equation which we often call as the Schrodinger equation itself right. This is the Schrodinger equation for the time evolution operator.

This is in the interaction picture and this is nothing but HU. So, this is very similar to how we write the time evolution operators Schrodinger equation in the Schrodinger picture except for the fact that here this is the interaction picture Hamiltonian right. So, this is just the transformation of the interaction part or off the correlation part. So, that is the only one which is being focused upon in the Dirac picture or the interaction picture.

Now here you have the time derivative of the time evolution operator the partial derivative with respect to time. This partial derivative is given by HU, so that is the HU write here instead of the derivative del U by del t. So, instead of del U by del t, I put in HU, I have included the ih cross which was sitting here okay. So, that has been included and the right hand side on the top is now read written as this.

Now put the limit t = 0 okay, we have already taken the time derivative that is what gives us HU right. Now put t = 0, so this t will go to 0, this t will also go to 0. So, let us do that, so now you have this t = 0, this t the second parameter is the start time which is minus infinity and you do the same in the term in the denominator. So, this is now taken care of and this right hand side is nothing but E - E0 as we saw from the Gell-Mann and Low theorem.

In other words E - E0 can be written as the limit alpha going to 0 of this expression. So, we have just written a consequence of the Gell-Mann and Low theorem in a form which we will find extremely useful to deal with these correlation terms. Now it is going to get messy before it becomes better. But you will see how that happens okay.
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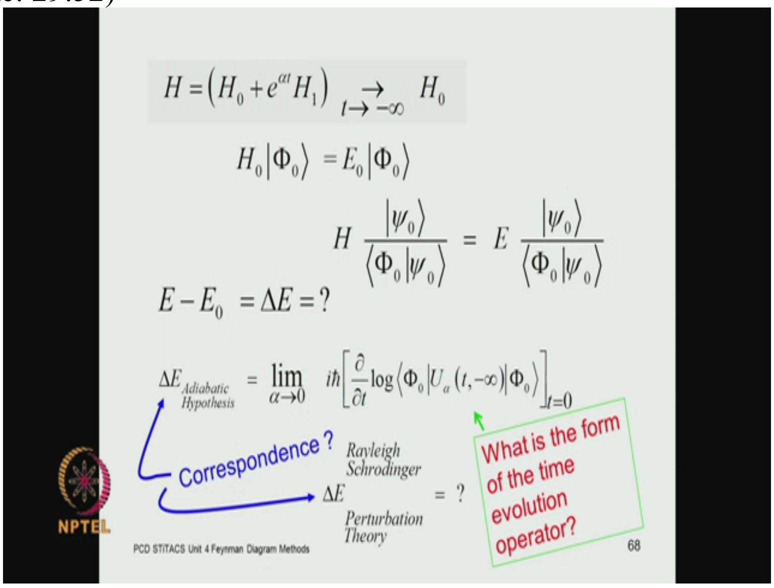

So, this is what we have got from the Gell-Mann and Low theorem, this is the energy difference in which we are interested. We have got an expression for this difference which we got in the previous slide which is given by this result but how do we get this is result. We got it from the Gell-Mann and Low theorem, we got it from the adiabatic hypothesis, we got it from the mathematical construct of the parameter alpha.

What do we expect it to correspond to; we expect it to give us information about whatever was missing from the unperturbed Schrodinger equation from the H0 right because that is the problem that we solved. We expect this energy difference to correspond to that, so in some sense we expect it to correspond in the perturbative sense to what perturbation theory would give us.

If we were to take into account the correlations which are missing in the term H0. And H0 problem is solved; it is the H Eigen value equation for the full Hamiltonian which is not solved. So, we expect it to correspond to what we get from the usual perturbation theory which is what I shall refer to as the Rayleigh Schrodinger perturbation theory. Because that that is the common form of the perturbation theory that we work with.

So that is the usual rarely Schrodinger perturbation theory and we expect some sort of a correspondence between the energy correction Delta E which we have got from the adiabatic hypothesis using the Gell-Mann and Low theorem and we will like to ask what exactly is this correspondence and how do we relate these terms in the perturbative sense it does not mean that we are using perturbation theory we are not.

If we were to use the Rayleigh Schrodinger perturbation theory in its raw form the way it is constructed in introductory courses in quantum theory that will not give us any result which will converge. And that is the reason you cannot approach, you cannot use that approach, you are not using the Rayleigh Schrodinger perturbation theory.

But in the perturbative sense the results that you are going to get will correspond to how you would get information about this part of the solution to the problem which is missing in the problem which has been solved. Which is the problem for the unperturbed hamiltonian H0. So, our correspondence will become clear when we analyze the time evolution operator because this is the most important creature here.

We have to get its expectation value in the unperturbed Eigen state in the Eigen vector of the unperturbed Hamiltonian. And the form of the time evolution operator has now to be studied in some details because that is where all the correlation is sitting okay.
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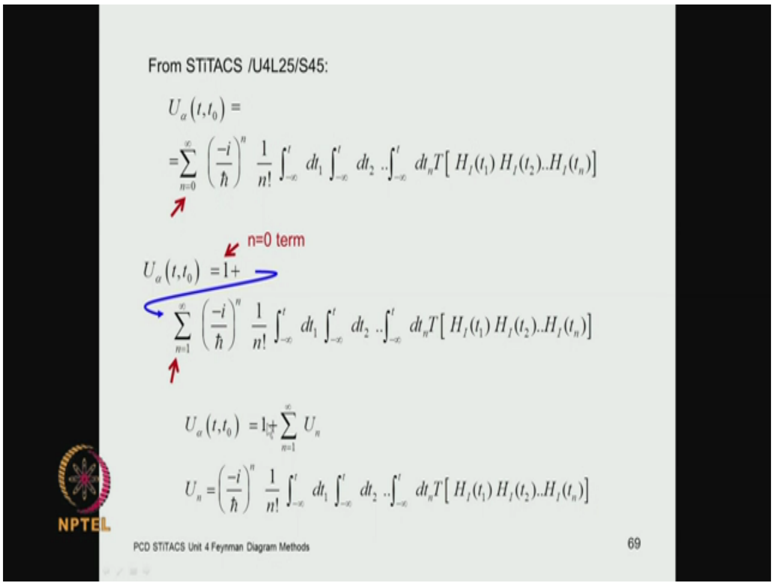

Now we did this in not the previous class but in the class before that, so that was in lecture number 25. So, and I am borrowing a result from that lecture which is on slide 45 of that lecture okay. That the time evolution operator was written as infinite terms if you remember but we rewrote those infinite terms as an infinite series okay.

If n going from 0 through infinity of this and the order in which these operators come is determined by this chronological order, chronological operator t. So, these operators are all time ordered which means that operators containing the latest time stand to the left okay. So, that is the chronological ordering that the t operator guarantees. So, that is the result that I am now going to use.

And we have obtained this result in some detail in the 25th lecture of this course okay. So, let us look at these terms there are infinite terms I separate the first term corresponding to n = 0 which is nothing but the unit operator. And then I have the remaining terms which, so what is being summed over is the same except that the summation is now going from n = 1 through infinity because n = 0 term has been separated out.

So, I first separate out the n = 0 term. So, now I write this time evolution operator as a sum of the unit operator plus again an infinite term but n going from 1 through infinity and what is being summed over is this Un okay. Now this is where all the correlations are setting in.

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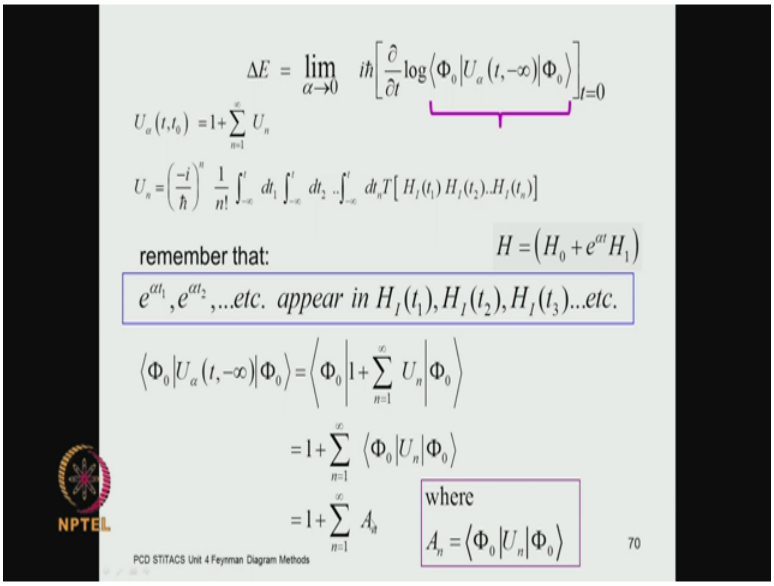

And this is where they will show up and if we can evaluate this term then we will get the term delta E that is the quantity of interest. So you have the time evolution operator U alpha which is the sum of this 1 + these remaining infinite operators over you remove 1 from infinity you still have infinite terms and there is nothing I can do to help you with that okay, so one would think that okay.

When you remove something we will have to deal with less but that is not the case it always alright. And I am really sorry I cannot help you with that. So, you have got this full Hamiltonian and these interaction picture Hamiltonian of the correlation part has got these e to the alpha t terms. So, this mathematical constructs e to the alpha t they are all sitting there in this.

So, in a HI t1 which is here you will have an e to the alpha t1 sure you have HI t2, so in HI t2 you will have an e to the alpha t2 okay. So, you will have this e to the alpha t term several places actually n places in each one of these from HI t1 right up to HI tn set all of these n places you will have these alpha parameter exponents. And then of course that is not being enough you of course have a summation over n going from 1 through infinity.

So, there is a lot to deal with okay. Now let us look at this expression now, subsequently we will have to take the logarithm and so on but let us just deal with this expression for the time being piece wise okay. So, let us look at this expression, you separate the first term the first term is nothing but the inner product of Phi 0 with itself, it is the norm of this state and let us say that this state is normalized so you get unity from here.

And then as some of these expectation values of Un and each Un is this. So, this matrix element is now what I call as An. Now you will; you might wonder why are we introducing new symbol, we already have those expressions and if you did not do that you are going to have to work with terms which are already cumbersome and you can only make them more cumbersome by expanding your notation.

So, this is just some strategy to save the ink that you would use to write in your notebooks okay. So, these are compact terms, so and you will see you will see this very soon, we are heading toward it. So, you have this An which is the expectation value of Un all right okay.
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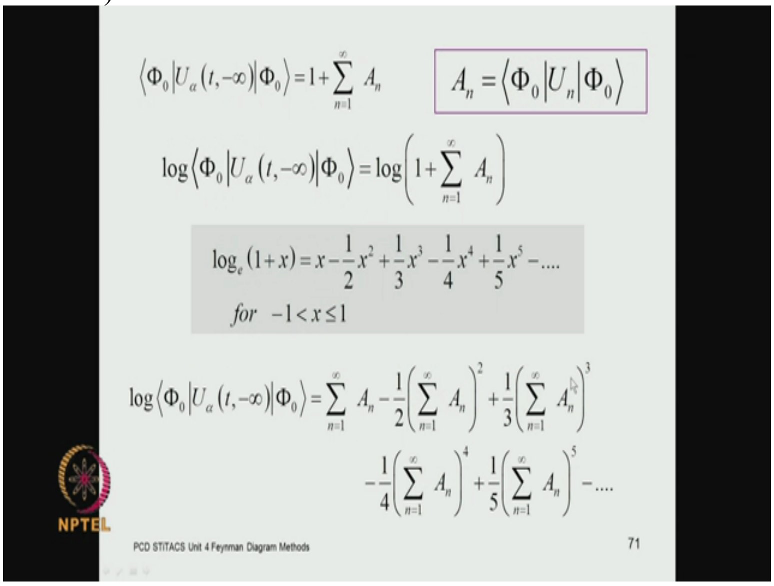

Now you have to take the logarithm of this okay, this is just the expectation value of the time evolution operator what about the log. Now this is the logarithm of 1+ another quantity. But this is a small quantity what is it made up of? It is made up of these U's, what are these U's made up of? It is made up of the correlation which was left out in our earlier problem. But our contention was that we have done most of the problem.

And it is a tiny thing which is left over right and we are worried about this tiny thing. So, the only thing we know about it is that it is a tiny thing. So, it is nothing but an expression similar to logarithm of 1+x where x is a small quantity. And this power series expansion is no, so we can use that result okay. So, let us plug it in and now you see how many terms you have, infinite terms.

You already have various are other kinds of infinities in our analysis and you have some more okay because now you have got infinite terms in the expansion of the logarithm term. Now I am sure you do not want to write the right-hand side over here instead of An okay. Here you have the square you have got the quadratic terms and then the cube and the fourth power and the fifth power and the six okay. So, you have infinite terms over here.
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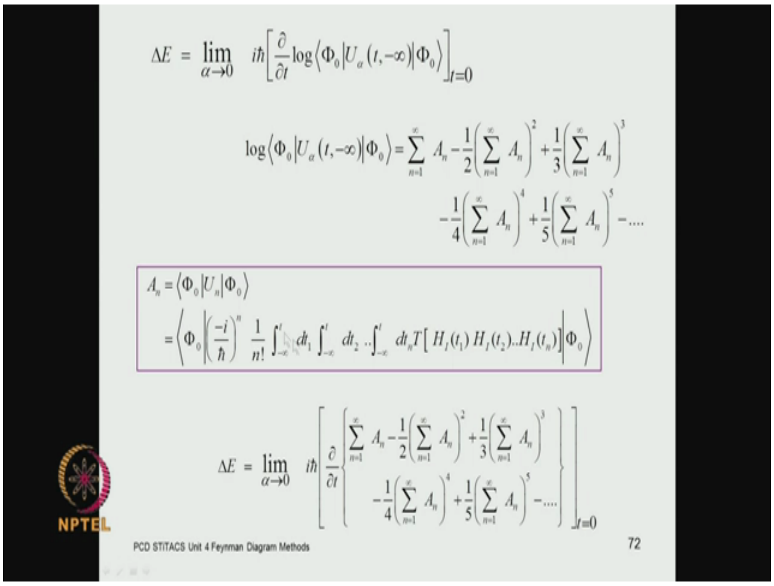

So, let us look at this result now you have got these infinite terms n going from 1 to infinity each An is so very compact creature it is nothing but the expectation value of the operator Un. But the operator Un itself has got a very complex structure okay. So, this is a lot to worry about.

So, now this is what we get for delta E, delta E is the result that you will get after you take the limit alpha going to 0 of ih cross. Then the time derivative of this logarithm functions, so you have got the time derivative operator here. And for this logarithm expression you now have these infinite terms which are in this beautiful bracket.

You put take the time derivative of everything that is there in this beautiful bracket put that in a square bracket like a box bracket and then take the value of the box bracket, the rectangular bracket at t = 0 and then you take the limit of alpha going to 0 right. So, that is what we are going to do now.

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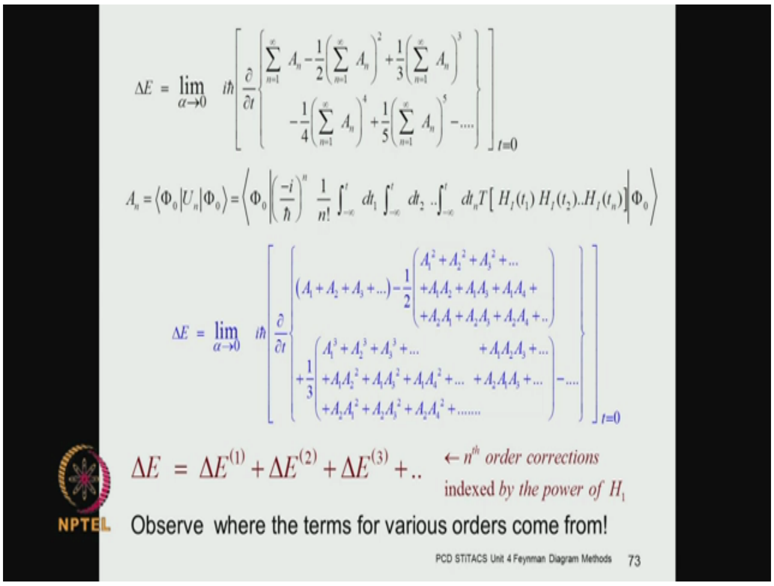

So, these are the terms that we have to worry about. Now let us write these summations, infinite terms An. So, An summed over n going from 1 through infinity, so you got A1 + A2 +A3 and so on. Now this is the square of a sum of these terms, so what will you have you will have quadratic terms.

You will have even A1 square, A2 square, A3 square and so on. You will also have A1 A2, A1 A3 and A1 A4, you will also have A2 A1, A 2 A3, A2 A4 and so on right. And you really have to keep track of each one of these terms. Because it becomes senseless to take the quadratic terms in A1 square and ignore A1 A2 because they are of the same order. It makes no sense to take account of A1 A2 but not A2 A1.

It is of the same order it becomes even trickier when you deal with the cube. So, here you have got A1 cube A2 cube, A3 cube but then you have got a third order term coming from A1, A2, A3 but you also have a third order term coming from A1 and A2 square and also from A2 and A1 square. So, there are all kinds of permutations which are possible okay and we have written terms only up to the third order and only some of the terms.

And then you have to take the time derivative and once you take the time derivative then take the value of the derivative at t = 0 and then you take if you are still alive right then take the limit alpha going to 0 right. Now you can write the expression delta E when you take all of these terms carefully as a sum of contributions from first order terms second order terms and the order is what I indicate by this superscript okay.

And these are in various powers of H1 which is the correlation term okay and these correlation terms become progressively small but that does not mean that you have conversions. And that is the essential reason why we are developing these alternative techniques. So, notice that various order terms come from different terms like second order terms I showed you from A1 square but also from A1 A2 and also from A2 A1.

Third order terms from A1 cube A2 cube but also from A1, A2 and A3 also from A1 A4 square right. So, the third order terms from you know different combinations of a linear term and a quadratic term or a product of three linear terms okay and so on. So, all of this has to be kept track off.

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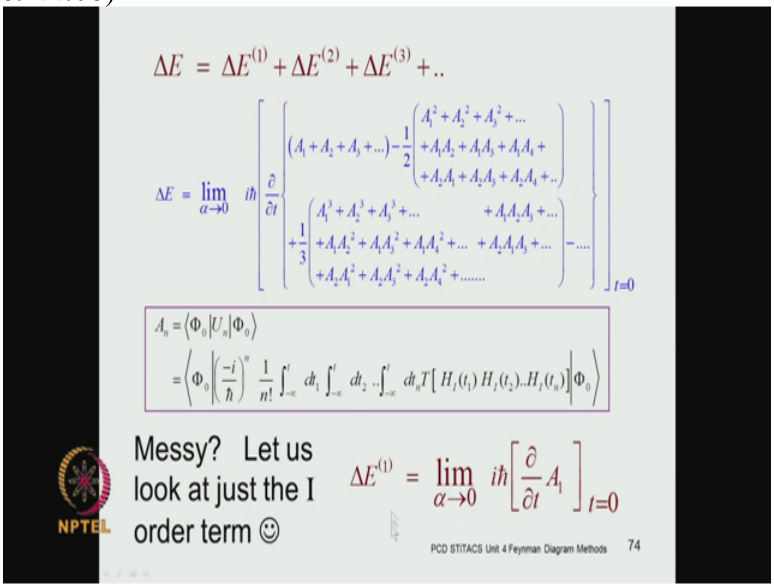

So this is your energy correction, now this is the sum and substance of what we have got okay. So, it is a friendly complex structure and it is a lot of mess, is it. It is a lot of mess. And let us see if we can look at just the first order terms to begin with okay so, always from the simplest to the more complex.

From the known to the unknown I got it right this time like alright. So, from the known to the unknown and from the simplest to the more complex terms, so we will begin with the first order terms and the first order term you have limit alpha going to 0, ih cross del over del t of let us say; let us deal with just the A1 term okay. Just to look at that.

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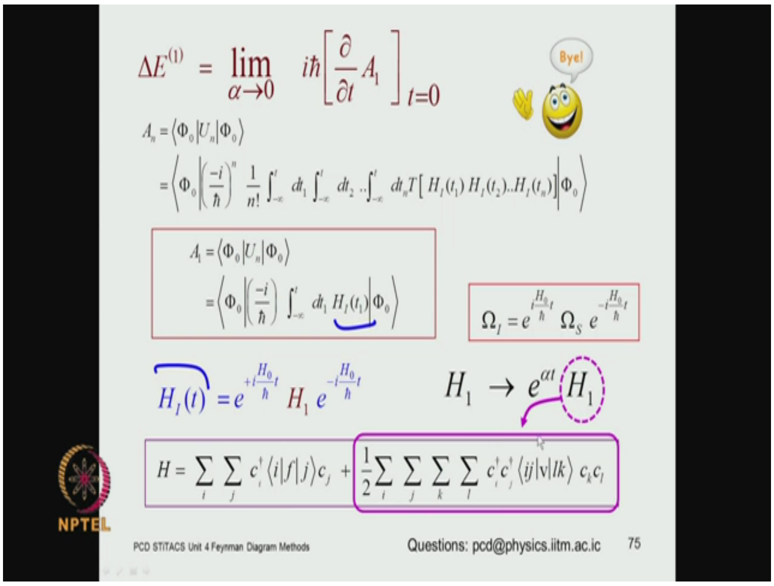

So, let us see how we are going to deal with this term. So, this is what your An in general is therefore we know what A1 is. A1 is just out of these n terms you have only one which is this HI at t1 there is only one time though to worry about in the nth term you have got n different instants of time to worry about t1, t2 up to tn. What you have over here is a chronological time ordered product of these operators.

For n = 1 there is only one instant of time that you are working with which is this t1 and this is the dummy variable which gets integrated out from the start which is minus infinity up to the current time t. Whatever it is and after doing this integration you can then take the derivative of this term with respect to time.

And then take the value of the derivative at t = 0. Now, this is the relationship between the interaction picture operators and the Schrodinger picture operators. The evolution that the transformation is through the unperturbed Hamiltonian H0, so that tells us that this HI at t1 this is the interaction picture term, is the transformation of H1 using this evolution operator, the transformation operator which contains the unperturbed Hamiltonian H0.

This is the term which will go in over here and what is this H1 now that is something we do know in terms of the creation and destruction operators okay. In the earlier unit in which we did second quantization, we wrote the electron-electron interaction term in terms of the creation and destruction operators.

So, you had one particle of terms which are over here and I am sure you remember this form of the Hamiltonian which we discussed in our earlier discussion on second quantization okay. So, in the second quantized form we have written the full Hamiltonian now. You have got the one electron terms and then you have the two electron terms. So, this is your operator H1. But we are going to have to deal with this put this in our expression for A1.

And then make up further; we have to progress further and then see how we are going to work with the second order and higher order terms. So, you see what a mess it really is and this is where the Feynman diagrammatic methods become handy. Those are the ones which I am going to introduce in the next few classes okay. So, now I think we have the basic machinery ready.

So, we have to; we are our interest is in getting delta E not just the first order but to higher orders as well. We could not get it using the Rayleigh Schrodinger or perturbation theory. So, I am going to stop here for today's class and we will proceed from this point in the next class. We have the electron-electron term, so this is the difficult part of the Hamiltonian. This is the unfriendly part as we have been referring to.

This is the one which is responsible for correlations the static average gives us the Hartree Fock which is the time independent Hartree Fock right. So, that we can get from which is equivalent to first-order Rayleigh Schrodinger perturbation theory which converges only for the first-order but for higher orders it does not. So, this is the H1 part this is the difficult part of the Hamiltonian.

With the difference that we have now scaled it by this factor e to the alpha t which is our mathematical device, so our Hamiltonian is not just this term plus what is in this purple block this is the Western colour is it not. So, this is this is in the purple block, this is the interaction term H1.

It is more of that it has been scaled by this mathematical construct e to the alpha t which is the adiabatic hypothesis which goes into the Gell-Mann and low expression which we have used. So, I will take the discussion from this point in subsequent classes. Yes (Question time: 49:56) in the last line we have the explicit expression A1 in the red box, so there the alpha dependence is we miss it or in the same slide 75th.

Yeah, the H1, there is a alpha dependence right, this HI t, this HI t1 is what you will get by simply transforming from the Schrodinger picture to the interaction picture. So, we are doing two things over here one is carrying out the transformation from the Schrodinger picture to the interaction picture but there is something more that we are doing.

And that is the adiabatic hypothesis which is why H1 which is in this first purple box is to be replaced by that term scaled by this e to the alpha T so when we are going to work with these correction terms in A1, A2 and higher order terms. We will bring in the alpha with every time there is a correlation term which is to be addressed. In fact that is the; that is the point I was anticipating in one of the previous slides.

Let me go back to the just to emphasize islets if I can quickly find it here yeah I alerted you to the fact that you have got in this Un in the nth term n number of different instants of time parameter. You have got a t1 here at the t2 here and a tn here but associated with each of these there will be an alpha parameter. So, you will have an alpha t1 you will have an e alpha t2 and so on right.

So all of these terms will have to be plugged in when we evaluate these terms carefully. So, just keep this at the back of your mind and then we will put in all these terms together. So we are doing you know more than just the Dirac picture. The Dirac picture is the basic platform that we use.

And over and above this Dirac picture in which we can do quantum theory we are now doing the adiabatic hypothesis which is the insert, which is the insertion of this mathematical device which is the e to the alpha t which we can use to let the Hamiltonian, the full Hamiltonian at t = 0 evolved from the unperturbed Hamiltonian at t going to minus infinity.

So that solution is known to us at t going to minus infinity from that Eigen state we want to get the Eigen state of the full Hamiltonian at t = 0 which is the now moment. So, that is where the alpha parameter comes in and it will of course be inserted not just for A1 but for every order term and there will be several terms.

Like with each of these time parameters t1, t2 and tn there will be an e to the alpha t1, e to the alpha t2 and so on. So, save this consideration in the back of your mind you want to need it in one of the next classes. I do not know if it will be the very next class or the one after but we are going to need it soon okay. And you see what a mess all this is and this is where the Feynman diagrams come in handy.

Because instead of dealing with so many terms, there you have to do the integration there are the Volterra type of integrations then you have the chronological operator you have to take the logarithms okay. You have infinite power expansions now instead of all of this if you were to work with just pictures what is not be nice okay.

Some fun diagrams and that is what we will be discussing in the next few classes okay. So, thank you all very much and we will take it from here in the next class.