

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 26
Dyson’s Chronological Operator

Greetings, so in our last class in this unit in which we plan to introduce Feynman diagram methods. We develop the equation of motion for the time evolution operator and today we will introduce the Dyson’s Chronological Operator. Now it will take us a few classes of you know development of the interaction picture formalism before we actually introduce these beautiful diagrams which are known after Richard Feynman.

So, that will come towards the end of this unit or at least after we are half way through. So, I believe there are some 6 or 7 classes in this unit.

(Refer Slide Time: 01:00)

$\psi_I(\vec{r}, t) = U_I(t, t_0) \psi_I(\vec{r}, t_0)$ Time evolution of interaction picture states

$H_I(t) U_I(t, t_0) = i\hbar \frac{\partial}{\partial t} U_I(t, t_0)$ ← Equation of motion for the time-development operator.

Differential equation for the Time Evolution Operator

Formal solution →

$$U_I(t, t_0) = e^{+i\frac{H_0}{\hbar}t} e^{-i\frac{H}{\hbar}(t-t_0)} e^{-i\frac{H_0}{\hbar}t_0}$$

Today:
we develop an integral equation for the time development operator

NPTEL PCD STITACS Unit 4 Feynman Diagram Methods 29

So, this is how an interaction picture state evolves with time or we discussed this in the previous class. The time evolution operator satisfies an equation of motion which is often called as the Schrodinger equation for the time evolution operator. And we got its final solution in our previous class which consisted of these 3 operators and you have to remember that you have H0 here, H0 here as well but the full Hamiltonian here.

So, H0 is the soluble part of the full Hamiltonian and the full Hamiltonian H is made up of the soluble part H0 and an additional part which we wrote as H1 which is the one which generates the complication. And which is make which is what makes the whole problem so complex.

So, we had the equation of motion set up for the time evolution operator and we have a formal solution in which the Hamiltonian appears in these 3 locations here as H_0 which is the soluble part of the Hamiltonian. Here we have the full Hamiltonian and here again we have the soluble part of the Hamiltonian.

So, the part which is missing in H_0 is the one which is generating correlations and that is not amenable easily to perturbation theory which is why we need many body techniques to handle that. Now what we are going to do today is to develop an integral equation for the time development operator because you can set up the equation of motion either as a differential equation as you see over it over here or as an integral equation.

And what we are going to do today is to develop an integral equation for the time development operator. So, mind you I have added a subscript i to remind us that this is the interaction picture time evolution operator.


(Refer Slide Time: 03:13)

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H_I(t) U(t, t') \quad \equiv H_I(t) U(t, t')$$

Raimes
 – *Many Electron Theory*
 Eq. 5.32 page 97

Fetter and Walecka
 – *Quantum Theory of Many Particle Systems*
 Eq. 6.17, page 56


$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H_I(t) U(t, t_0)$$



PCD STITACS Unit 4 Feynman Diagram Methods 30

And the primary references are these two books Raimes and Fetter and Welecka. The notation is slightly different in the two books here you have t and t prime whereas Fetter and Welecka. You have t and t_0 but other than that you know it is; the both the books provide you essentially the same kind of treatment.

(Refer Slide Time: 03:38)



$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H_I(t) U(t, t_0)$$

i.e. $\frac{\partial}{\partial t} U(t, t_0) = \frac{-i}{\hbar} H_I(t) U(t, t_0)$

integrating from t_0 to t :

$$\int_{t_0}^t dt' \frac{\partial}{\partial t'} U(t', t_0) = \frac{-i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$$

$$U(t, t_0) - U(t_0, t_0) = \frac{-i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$$

$U(t_0, t_0) = 1$

$$U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$$

PCD STITACS Unit 4 Feynman Diagram Methods 31

So, this is the time evolution operator. So, which this is the differential equation for the time evolution operator. I just take $i\hbar$ cross on the other side and now you have got a derivative on the left. So, it is obvious that it is amenable to integration, so integrated from t_0 to t . And on the left hand side now you have an integral of a derivative.

So, you can immediately integrate this put the limits and you have the difference of U at the upper limit and the lower limit. So, the lower limit is $U(t_0, t_0)$ when $t' = t_0$ and at the upper limit you have got $t' = t$. So, this difference is equal to this definite integral okay. So, it is a definite integral from a lower limit to an upper limit and this is the equation that you will satisfy.

Now we already know that the time evolution operator from any instant of time to the same instant of time is essentially the unit operator. So, you take this unit operator to the right and you get the solution for $U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$.
(Refer Slide Time: 05:14)

$$U(I, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$$

Independent variable t appears as UPPER LIMIT
 If U were ordinary functions, then such integrals would be "VOLTERRA INTEGRALS"

$U(t, t_0) \rightarrow$ time development operators
 \rightarrow not ordinary functions of time t

Iterative solutions available; which are guaranteed to converge in the case of ordinary functions
..... we attempt similar procedures in the present case.

We are dealing with operators....
....so we must preserve the 'ordering'

NPTEL
 PCD STITACS Unit 4 Feynman Diagram Methods 32

Now this is nice but in some sense it is a solution in another not really so because you always a solution means that you are able to determine the left hand side in terms of the right hand side. And how can you get the right hand side because the left hand side involves the U which is the left hand side under the integration okay. So, it formally correct but it really is not very helpful.

So, we are still stuck and we still have to figure out how we are going to resolve this okay. So, it is formally absolutely correct nothing wrong with it but not very helpful at this point. So, we still have to figure out how we are going to deal with this. There is a rather issue over here that if you look at the upper limit of integration over here.

It is also an independent variable time is the independent variable over which integration is carried out. And it appears as an upper limit of the integration over here. So, these integrals are well known in mathematics and typically they are known as Volterra integrals. In which the independent degree of freedom over which the integration is carried out appears as one of the limits of integration.

And the mathematics of Volterra integrals is fairly well developed and those techniques can be used by large you can solve this especially when the; what is being integrated are functions. We have to be a little extra careful in quantum theory in physics you do rigorous mathematics as I always like to point out but you do something more than that.

Because the mathematics that you are doing has to conform to the physical laws of nature and in physics the relationship that we are working with involves not ordinary functions but operators. So, the operator algebra will have its own consequences and the immediate

consequence that concerns us in quantum theory is that when you are working with operators we never take for granted that when you have two operators A and B they commute.

They sometimes they do and sometimes they do not. So, we have to be very careful about it. So, for ordinary functions iterative solutions for such equations can be well developed. These are the Volterra integrals and they methods are available for that. In the present case very similar solutions some similar strategies can be developed and that is what we are going to do in today's class.

But the inspiration comes from the mathematical formalism which is well developed and very well organized already and we will keep an additional rider on in our mind that we must preserve the ordering okay. So, the order in which the operators come that has to be very carefully kept track off and that is something that you do not always have to do when you are dealing with ordinary functions.

(Refer Slide Time: 08:45)

$$U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' H_I(t') U(t', t_0)$$

$$U(t', t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t'} dt'' H_I(t'') U(t'', t_0)$$

$$U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' H_I(t') \left[1 - \frac{i}{\hbar} \int_{t_0}^{t'} dt'' H_I(t'') U(t'', t_0) \right]$$

$$U(t, t_0) = 1 + \left(\frac{-i}{\hbar} \right) \int_{t_0}^t dt' H_I(t') + \left(\frac{-i}{\hbar} \right)^2 \int_{t_0}^t dt' H_I(t') \int_{t_0}^{t'} dt'' H_I(t'') U(t'', t_0)$$

Observe →

So here is the solution this is the formal solution and this one will have a very similar solution but now the variable t prime is the dummy variable which is used in the first equation. So, when you want to use a dummy variable for which will appear in the integration for U t prime t0, you must use a different dummy variable.

And the one that I have used is t double prime okay. So, I have U t prime t0 which is given by an exactly identical relation with the difference that now the integration is over t double prime and the integration is over the limits t0 to t prime which are the two parameters which come here okay.

Over here the integration was over t' which was the dummy label here and this was from this limit t_0 which is the lower limit to this one which is the upper limit coming over here. So, now you have $t' = t_0 = 1 - i$ over \hbar cross integral t_0 to t' and if you now put this the second equation in the first okay then the left hand side which is $U(t, t_0)$ is now given by $1 - i$ over \hbar cross.

And now you have these terms so you have $dt' H(t')$ and in place of this you can write this okay. Now it is not necessary to really take notes and write these equations in your notebooks during the class because at the end of the class all of this is going to be uploaded a PDF will be uploaded on the course website, so you will have access to that.

So, you do not have to really write down anything just follow the discussion and see how the steps are developed and that is part of the reason I use these slides. So, that you can have all the material you do not have to write down anything in the class and you can concentrate on how the development of the formalism takes place okay.

So, if you have any question you can always stop me but otherwise just follow the discussion all right. So, now let us write these terms, so you have got the first term which is here, you have got the second term coming from this and then you have got a unit operator here which does nothing really. So, the second term is $-i$ over \hbar cross this integral t_0 to t dt' and then you have this $H(t')$ over here right, so that is the second term.

What about the third term? You have got $-i$ over \hbar cross coming twice, so you get the square root of $-i$ over \hbar cross. You have got two integrations 1 over t' the other over t'' and the limits of t' are t_0 to t . So, that is what you have over here, the limits of t'' are t_0 to t' and then what is being integrated out are a $H(t')$ and a $H(t'')$.

So, $H(t')$ comes first and $H(t'')$ on its right. So, that order has to be maintained okay and then this U is also an operator so this comes at the end okay. So, the ordering of the operators must be respected you cannot swap them these are quantum operators okay.

So, let us write them in a slightly neater form, so you have got the integration over t' integration over dt'' then you have got a $H(t')$ over here, $H(t'')$ and $U(t'', t_0)$. So, all the orders are written in the correct sequence the integration limits are taken care of and this is the form that we will analyze now.

Observe however that you have got U, so this is again not really a solution because you will have a similar expansion which is written in the very first equation in the top of the slide which will appear over here okay. So, you will actually end up getting an infinite series and then you can develop some approximation methods to see if you can truncate it somewhere okay.

So, essentially you will you are looking at an infinite set of series. So, just remember what is at the left and what is it the right. So, $H_i t$ prime is at the left $H_i t$ double prime is at the right. (Refer Slide Time: 13:42)

The slide contains the following mathematical content:

$$U(t, t_0) = 1 + \left(\frac{-i}{\hbar}\right) \int_{t_0}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') U(t'', t_0)$$

$$U(t'', t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t''} dt''' H_I(t''') U(t''', t_0)$$

$$U(t, t_0) = 1 + \left(\frac{-i}{\hbar}\right) \int_{t_0}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \left[\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') \right] + \dots$$

Consider the 3rd term

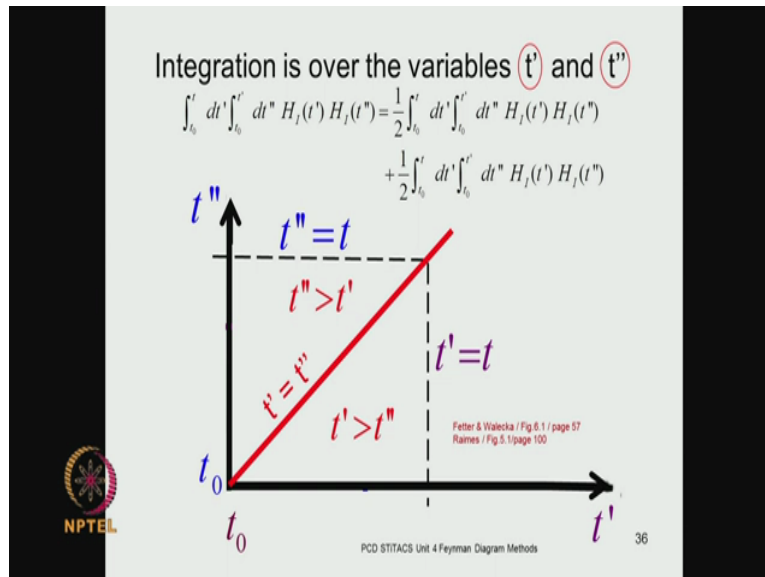
$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') = \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') + \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t'') H_I(t')$$

NPTEL
PCD STITACS Unit 4 Feynman Diagram Methods
34

So, that is what I bring to the top of this slide here now and here you will have a similar expression. So, now you have another integration a third dummy variable which is t triple prime and we keep showing this for the rest of the course and never finish because there are infinite jumps right. So, what we will do is represent the remaining terms by these dots okay. That is the tail of the infinite series all right.

Now in this infinite series you have got a first term, a second term, a third term and then the fourth term and the fifth and so on all the way to infinity. Now we look at the third term and the third term does not have this U okay. So, the third term we can certainly discuss by itself okay. So let us look at the third term and any physical quantity is the sum of two of its halves okay. So, I write this term and take half of it.

And write the same term take the half of it and add these two okay. Now this; will really, this is a simple thing that we are doing but it is going to give us the tools to write this whole term in a very beautiful manner and you will see it in the next few minutes. (Refer Slide Time: 15:30)

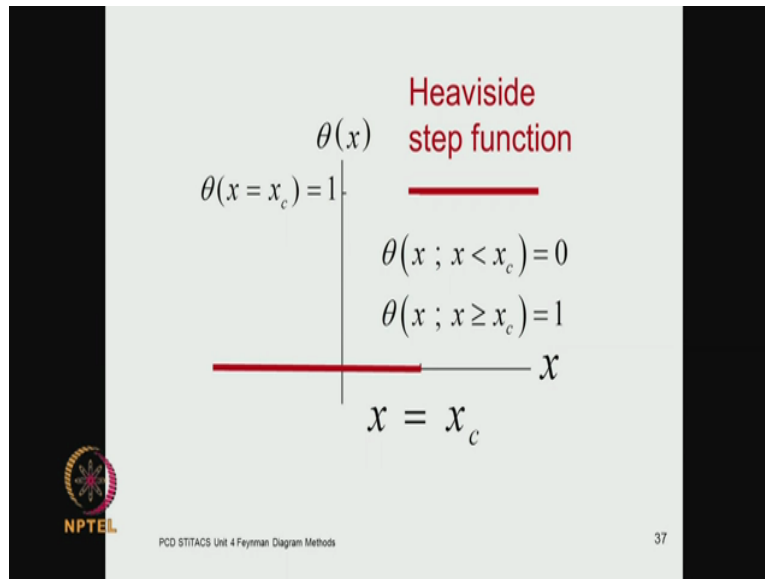


So, these are the two halves which we have added together to get the left-hand side this is the third term other than that - i over h cross and so on right. So, this is the integration part of it, the two integration variables t' and t'' both our time variables but they are quite independent of each other and they are to be treated like independent variables. They are completely independent degrees of freedom.

And you can represent them by two variables which you represent graphically orthogonal to each other. Orthogonal because they are completely independent of each other okay, so you have got t' on the x axis t'' on the y axis and you have the t_0 at the crossing which is the origin of this orthogonal Cartesian kind of coordinate frame of reference for time both are time one is t' the other is t'' .

If you look at a diagonal in this along this diagonal the variable t' is equal to t'' along this diagonal. Above this diagonal t'' is greater than t' and below the diagonal t' is greater than t'' is the other way around right. You can also look at some special points like a particular value of t when $t' = t$ is given by what happens on this vertical line right.

So, this vertical line corresponds to $t' = t$ and likewise you have a horizontal line over here at which $t'' = t$. So, this is a very simple neat graph you will find it in both the books by Raimes as well as Fetter and Walecka and all it does is to describe how these two variables are dealt with as if they are completely independent of each other. And what consequences we have on the integrations that we are considering in these two terms. (Refer Slide Time: 17:40)



And to do that we make use of what is called as the Heaviside step function and you have probably met the Heaviside step function earlier so let me remind you. It is a function whose value is zero for an independent parameter up to a certain point and beyond that point its value is equal to 1. So, he surely jumps there is a singularity it jumps okay.

It jumps and that is the reason it is called as a step function it is just the way you climb a staircase okay. So, this is called as a step function and we will use the Heaviside step function to represent our operator functions in the integrant.

(Refer Slide Time: 18:26)

$$\int_{t_0}^{t'} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^{t'} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') + \frac{1}{2} \int_{t_0}^{t'} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'')$$

$$\int_{t_0}^{t'} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^{t'} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t'-t'') \quad t_0 \leq t'' \leq t'$$

NPTEL Fetter & Walecka / Eq.6.21 / page 57 PCD STITACS Unit 4 Feynman Diagram Methods 38

So, this is what we are integrating out and in this term for example t double prime must go from t0 to t prime okay. So, it shows a certain order in the variable t double prime because t double prime must always be greater than or equal to t0 the lower limit of integration. And it must always be less than or equal to t prime which is the upper limit.

And if this relation is not satisfied then what is being integrated out should be considered to be 0. So, you can use the Heaviside step function to represent to this. Because the Heaviside step function will have a value which is 0 below a cut-off and it will be unity above that cut off okay, so, let us do that.

Let us write, so there are two terms on the right side and the first term I write using the Heaviside step function and what it will let me do is allow me to take this upper limit t prime to t because I do know that I have to carry out another integration over t prime which must go from t0 to t right.

So, this limit will have to be stretched all the way up to t so I extend this limit t prime to t but I have to respect the fact that t double prime must always be less than or equal to t prime because that is the integration constraint which is coming from these limits. So, I have a Heaviside step function over here so let me make it manifest here. And this Heaviside step function will take care of this and allow me to extend the integration.

The top limit of the integration from t prime to t, so now we have got the first term which is strictly correct it is exactly in accordance with this exactly in accordance with the find that t double prime varies from t0 to t prime and furthermore that t prime varies from t0 to t okay. Because the upper limit of integration itself is a variable this is what made it a Volterra integral in the first place if you remember okay.

There because they have the independent degrees of freedom appear as limits of integration. So, this is how you make use of the Heaviside step function which is theta and this will be unity if and only if t prime is greater than t double Prime okay. So, that takes care of it. (Refer Slide Time: 21:27)

$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t'-t'') + \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'')$$

$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t'-t'') + \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t'-t'')$$

$t_0 \leq t'' \leq t'$

$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t'-t'') + \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \theta(t''-t')$$

$t'' \leftrightarrow t'$
in 2nd term

Fetter & Walecka
Eq. 8.21 / page 57
PCD STITACS Unit 4 Feynman Diagram Methods 39

So, now you will have the first term in which the limits are properly taken care of. And now let us look at the second term which is the second half of the whole the whole is on the left side which we wrote as two halves. The first half and the second half we now look at the second half and is the second half look at the upper limit of t double prime, t double prime goes from t0 to t prime.

So, you have t double prime which must go from a lower limit t0 to an upper limit t prime which is this okay. And now you can let the upper limit go all the way to t because t prime must subsequently go from t0 to t, so you let that happen and then have the ordering taken by the Heaviside step function right.

So, now everything is fine and t prime and t double prime are dummy labels we can interchange them as long as you call you rename t prime as t double prime and rename t double prime as t prime you cannot blame me for that okay. But that is going to let you write these terms in a very nice manner okay, so that is why you do that. So, you now re-label t prime as t double prime and t double prime as t prime.

So, when you do that you have this relation so instead of t prime you have t double prime instead of t double prime you have t prime here. Instead of this t prime you have got t double prime here, instead of this t double prime you have got this t prime here and instead of the Heaviside step function t prime - t double prime.

You have Heaviside step function t double prime minus t prime. So, everything is exactly the same as before all we have done is to interchange the labels okay. (Refer Slide Time: 23:27)

Operators containing the latest time stand farthest to the left.

$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') = \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' [H_I(t') H_I(t'') \theta(t' - t'') + H_I(t'') H_I(t') \theta(t'' - t')]$$

T: Time-ordered product of operators.

Operators containing the latest time stand farthest to the left.

$$T \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') = \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' T [H_I(t') H_I(t'')]$$

Fetter & Walecka / Eq. 6.19 / page 57

$$U(t, t_0) = 1 + \left(\frac{-i}{\hbar}\right) \int_{t_0}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \frac{1}{2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') + \dots$$

Generalizing:

$$U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T [H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

Fetter & Walecka / Eq. 6.23 / page 58

NPTEL

41

PCD STITACS Unit 4 Feynman Diagram Methods

So, let us take it to the top now and what is interesting about this is the consequence of the Heaviside step function because that has got a discrete value which is either 0 or 1 depending on a cut-off of the argument of the Heaviside side step function. What it is essentially doing is preserving a certain ordering of the time operators.

What it ensures that the operator containing the latest time stands farthest to the left okay. These operators stand farthest to the left and it always reminds me of the orders they give in the Army or the NCC lumba thaye choda-bhaye eak line me kadhva have you heard of it okay.

Lumbathaye the tallest man stands to the right and the shortest to the left because otherwise when soldiers line up in one row and they have different heights it looks like a very crooked skyline. But if you order them to stand so then the tallest one is to the right and the shortest one to the left lumbathaye chota bhaye okay. Then it looks like a very neat ordering of how the soldiers line up okay.

That is how it is often done in the armies, so that your squad looks very nice okay. So, here you have the operators containing the latest time stands farthest to the left and that is ensured by the Heaviside step function. But you can do it by writing the same in a different way using what is called as the chronological operator or the time operator.

And what the time operator will do is that it will order all the operators on which it is operating such that the operator with the latest time stands farthest to the left okay, it is exactly the same order okay. And that is done by this operator which is called as the T operator. So, first we combine these two terms we have written half over here and you have got these two terms sitting over here.

And now we will exploit the fact that operators containing the latest time stands farthest to the left by introducing the T operator this is called as the chronological operator or the T operator sometimes as the Dyson's chronological operator and so on okay. And what this operator is going to do is whatever operators it operates on and these operators have time appearing in the argument okay.

So, you have what T' here and T'' and what this operator will do the T operator the chronological operator is that it will force these two operators to interchange their positions if need be, if it is required that the operator with a later time stands farthest to the left okay. And that is achieved by this time order operator the T operator. So, this integral you can write in terms of the T operators.

So, now instead of the Heaviside step function θ I have the same exactly the same effect which is represented by the T operator okay. So, I introduce the Heaviside step function as an auxiliary step but we do not really need it. What we need is the time ordering of these correlation operators that must be preserved and the Dyson chronological operator guarantees that it will be done.

And now you have you if you remember you had an infinite series the first term, the second term, the third term and then the rest of them represented by these dots. The third term was this which we wrote as two halves and what we find is that these terms can be combined in this manner by using the T operator. So, let us do that you can generalize this we had done this only for two operators.

But here you have to deal with this infinite series all these dots okay. So, you can generalize it and you can write all of these dots let n go all the way to infinity because those are the infinite terms which are sitting in these dots. You can let n go to infinity and you have a very general form of the solution okay. You have a very general form it is a very formal solution it is a complete solution, it is absolutely accurate.

What it requires you to do is to keep track of the time ordering of these operators you can let the integration variables go from t_0 to t like over here both t' and t'' went from t_0 to t . And here we have generalized it to all of these n integration variables t_1, t_2, t_3 all the way up to t_n and we then let n go from 0 to infinity every time you have got this $-i$ over \hbar cross.

But now you will have $-i$ over \hbar cross raised to the power n right. So, you have that taken care of over here. You do have to keep track of the time ordering, so you have got the T operator over here which takes care of that and because there are factorial n time orderings over here which are available.

You have to; over here you have divided it by 1 over factorial 2 , 1 over 2 as it was and here you have got 1 over factorial n because those are the number of you know different orderings that you can have. So, now you have got a very general solution in which the T operator has been made use of okay.

(Refer Slide Time: 30:05)

$$U(t, t_0) = 1 + \left(\frac{-i}{\hbar}\right) \int_{t_0}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') + \dots$$

T: Time-ordered product of operators. Fetter & Walecka / page 57,58
Operators containing the latest time stand farthest to the left.

$$U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

Now, let $t_0 \rightarrow -\infty$

$$U(t, -\infty) = 1 + \left(\frac{-i}{\hbar}\right) \int_{-\infty}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' H_I(t') H_I(t'') + \dots$$

$$U(t, -\infty) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

$$U(t, -\infty) = 1 + \sum_{n=1}^{\infty} U_n$$
 with

$$U_n = \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

PCD SITACS Unit 4 Feynman Diagram Methods 42

So, let us work with this now. You have got the solution this is what we had on the previous slide okay. We have all together, so we have this general solution. Now what we are going to do is let t_0 go to minus infinity because this relation is valid no matter what the values of t_0 and t are. So, we are going to let t_0 go to minus infinity we can let later let t go to 0 because we have;

We are introducing adiabatic switching in such a manner that the Hamiltonian is the soluble part H_0 at minus infinity and it is a full Hamiltonian at t_0 okay that is how we are developing the time evolution. So, we now let t_0 go to minus infinity, so all the lower limits which were written as t_0 over here are now written as minus infinity.

Look at it over here, look at it over here, look at it over here, all the lower limits are now minus infinity, so that is what we have done first. And here we have these dots for the infinite series but in an equivalent expression over here, we do not have these dots to represent the infinite terms instead we have a general term which is the n th term. And we let n go all the way from 0 to infinity.

So, these two are completely equivalent forms one in which we use these dots to write the unreturned terms. And in this lower equation we have an exactly equivalent solution of final formal expression for the time evolution from minus infinity to t in which the T operator the Dyson chronological operator is used and we now let n going from n to go from 0 to infinity okay.

So, these dots are replaced by this upper limit of the summation which is infinite and that is the role it has. Both the term both the expressions are completely equivalent and exactly

equivalent to each other. So, here you have got the sum going from 0 through infinity I factor out the term corresponding to $n = 0$ which is the unit operator.

And the rest of the terms I bundle up together as sum over U_n and going from 1 to infinity instead of 0 to infinity because the term corresponding to $n = 1$, $n = 0$ is already factored out over here. So you have got 1 plus this sum over U_n and going from 1 through infinity and U_n this general expression is what you have here which is $-i$ over \hbar cross to the power n 1 over factorial n .

And you have got these n integrals each from a lower limit minus infinity to an upper limit t and whether t_1 is greater than t_2 or not and what would be the relative ordering of these two operators is determined by this T operator the chronological Dyson's chronological operator which guarantees that the operator is containing the latest time will stand farthest to the left. (Refer Slide Time: 33:45)

T: Time-ordered product of operators.
Operators containing the latest time stand farthest to the left.

$$T[A(t_1)B(t_2)] = A(t_1)B(t_2) \quad \text{if } t_1 > t_2$$

$$= B(t_2)A(t_1) \quad \text{if } t_2 > t_1$$

$t_1 = t_2$: chronologically same!

$$T[H_I(t_1)H_I(t_2)] = H_I(t_1)H_I(t_2) \quad \text{if } t_1 = t_2$$

$$= H_I(t_2)H_I(t_1)$$

$$T[H_I(t_1)H_I(t_2)] = H_I(t_1)H_I(t_2) \quad \text{if } t_1 \geq t_2$$

$$= H_I(t_2)H_I(t_1) \quad \text{if } t_2 \geq t_1$$

$$\hat{T}[H_I(t_1)H_I(t_2)] = \hat{T}[H_I(t_2)H_I(t_1)]$$

NPTEL
 PCD STITACS Unit 4 Feynman Diagram Methods
 43

So, what does it do for two operators if you have two operators A and B one at t_1 and the other at t_2 and if t_1 is greater than t_2 then A will stand to the left of B. If t_2 is greater than t_1 that B will stand to the left of A okay that is what this operator is doing. If $t_1 = t_2$ is the same, so it really does not matter okay, so when $t_1 = t_2$ then the interaction term the correlation term the Hamiltonian $H_I(t_1)$ and $H_I(t_2)$ will be equal to this if $t_1 = t_2$.

And it really does not matter how you write them, so in general either for t_1 greater than t_2 or equal to t_2 okay this identity holds. So, both for t_1 greater than the t_2 as well as $t_1 = t_2$ and we will use this in the general expression. So, I show it for just two operators but you can do it for 3, 4 or infinite it is the same right. Now what is interesting as a consequence of this is that you have this general result.

I think there is a little font problem over here which is why I had a caret appearing on top of the T but look at the argument here, here the first argument is t1 and here the second argument is t2 on the right-hand side I have got the first argument which is t2 and the second argument which is t1.

But this operator T the chronological operator ensures that whichever is latest is going to stand on the left. So, it really does not matter if I write this as how it is written on the left hand side or how it is written on the right hand side because the T operator ensure the equivalence of the two is going to guarantee that whatever is the latest operator you know will stand to the left.

(Refer Slide Time: 35:50)

$$U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

Consider n^{th} term in this series:

$$\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

There are $n!$ 'time-orderings' of the time labels

t_1, t_2, \dots, t_n

one of these $n!$ ways is: $t_1 > t_2 > \dots > t_n$

t_1, t_2, \dots, t_n are dummy labels that get integrated out
and

$T[H_I(t_1) \dots H_I(t_i) \dots H_I(t_j) \dots H_I(t_n)] = T[H_I(t_i) \dots H_I(t_j) \dots H_I(t_1) \dots H_I(t_n)]$


T: Time-ordered product of operators.
Operators containing the latest time stand farthest to the left.

PCD STITACS Unit 4 Feynman Diagram Methods 44

So, we now look at the nth term which is this and there are how many factorial n time orderings take one of them. Any one of them let us take this one in which t1 is greater than t2 which is greater than tn okay. So, this is certainly one of the factorial n orderings that you may have. And if you take one of these then you just go ahead and stick it in. So, you write t1 t2 all the way up to tn in this particular order.

But then if you were to interchange it, like if you have the jth argument here and the ith argument here it would not matter because the chronological operator T would guarantee that the latest operator will stand to the left. So, just what we showed for the for just to operators also holds good for n even in the limit n going to infinity okay. So, we will make use of this now.

(Refer Slide Time: 36:51)



$$H = H_0 + e^{\alpha t} H_1$$
 A purple arrow points from the text "adiabatic switching control parameter" to the $e^{\alpha t}$ term in the equation above.

This mathematical device enables us use the provisions of the INTERACTION PICTURE very fruitfully.

α : small (positive) ; in the end $\alpha \rightarrow 0_+$

as $t \rightarrow -\infty$; $e^{\alpha t} \rightarrow 0$ & $H = H_0 \leftrightarrow$ soluble part

as $t \rightarrow 0$; $H = H_0 + H_1 \leftrightarrow$ full Hamiltonian

PCD STITACS Unit 4 Feynman Diagram Methods 46

And we turn on the perturbation adiabatically and that is where theoretical physicists have an edge over experimental physicists because experimentalist cannot switch on and off an interaction. Theoreticians represent that interaction by some term and they can develop an approximation in which they say that okay let me do it when this term is zero. And now let me do it when it is not zero I will just switch it on okay.

So that is a mathematical switch okay and mathematics lets you do that. So, you have got this perturbation H_1 which is the difficult part you do not like it because this is the one which makes the problem, you know you cannot solve the problem. We have argued number of times that if you are looking for exact solutions even nobody at all is already too many. You cannot get exact solutions you have to develop approximation methods.

There are these problems like in the many electron problem the atomic problem in which you have got n electrons you get a solution in the Hartree Fock formalism which is good. You have got a nice solution but that is not exact because it leaves out something. What does it leave out? It leaves out the electron correlation it takes into account the exchange correlations but it leaves out the Coulomb correlations.

And we are now going to worry about how to account for the Coulomb correlations. So, those are the ones that you cannot make use of; by you cannot handle using perturbation theory. We showed in some of the our earlier classes including in the previous unit that the Hartree Fock result is equivalent to what you would get if you were to treat the electron-electron interaction perturbatively, if you go up to the first order perturbation theory.

And at that point I had commented that if you do second order perturbation theory, if you try to get additional effects then the series does not converge. So pertabation theory does not

work. So, perturbative methods are not always successful okay. And that is the reason you have to develop these new techniques which is why we are getting into Feynman diagram methods.

And you have this unfriendly part which you cannot handle using perturbative methods perturbation series does not converge. And you have to find some mechanism to deal with this; this is the correlation part okay. This is what is left out of the Hartree Fock that is the one that we are trying to deal with. So, you have got a solvable part and you have got another part which is H_1 .

And what we do a theorist is to add a mathematical construct multiply this by e to the power αt . Now nature would not let you do that but mathematics lets you do that okay. But eventually what you do as physicist must correspond to nature because that is what physics is about right.

So, we develop this mathematical technique we multiply H_1 by e to the power αt okay. And in the end if we take the limit α going to zero then you get the full Hamiltonian which is what the problem really is okay. We are looking for solutions for the full Hamiltonian, so that is our target.

And we will get solutions to this problem by developing a formalism by inserting a mathematical device which is the switch control parameter. So, α is the switch, α is the adiabatic switch it is a mathematical construct and what it does is if you take the limit t going to minus infinity then the full Hamiltonian collapses into the soluble part that we are happy with because we know the exact solution for that okay.

So, in the limit we get in the limit t going to minus infinity α is a positive number okay. And we will let the limit α go to 0 while staying positive okay. So, α is some tiny positive number which will eventually find its limit which is 0. So, in the limit t going to minus infinity you have got the solution part of the Hamiltonian and as t goes to 0 you get the full Hamiltonian which is really the problem for which we are finding solutions.

So, now we have got a very nice mathematical device and we switch on the perturbation adiabatically in a very quasi-static manner just the way you do things in thermodynamics. And we are interested in end results such that they are independent of this mathematical device okay. And we take the limit are going to 0 okay.

So, this is the summary of what we have we have got a syllable part this we are happy with. We know the exact solution this is the full Hamiltonian that we want to address and this is the adiabatic switch which is the mathematical device to deal with this residual correlation which we are not able to handle in the Hartree Fock approximation. (Refer Slide Time: 42:41)

INTERACTION PICTURE

$\Omega_I = e^{\frac{iH_0 t}{\hbar}} \Omega_S e^{-\frac{iH_0 t}{\hbar}}$

$\psi_I(\vec{r}, t) = e^{\frac{iH_0 t}{\hbar}} \psi_S(\vec{r}, t)$


$$H_I(t) = e^{\frac{iH_0 t}{\hbar}} (H_1) e^{-\frac{iH_0 t}{\hbar}}$$

$$H = H_0 + e^{\alpha t} H_1$$

*adiabatic switching
control parameter*

Perturbation: 'unfriendly' part,
controlled by the mathematical switch

$H_I(t) = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iH_0 t}{\hbar}}$



PCD STITACS Unit 4 Feynman Diagram Methods 47

We are doing this analysis in the interaction picture in which the Schrodinger picture operators transform to interaction operators, interaction picture operators using this. And Schrodinger picture wave functions transform to the interaction picture wave functions using this relation. So, we discussed this in our previous class.

And in this interaction picture the correlation term the difficult part of the Hamiltonian in the interaction picture transforms to this but this was the actual interaction that we wanted to work with. But now the interaction that we have to work with is not just H1 but H1 times e to the alpha t okay. In our formalism we have now introduced this e to the alpha t.

So, let us plug this in and what do we get for the interaction picture Hamiltonian. See what the same kind of relation over here but this H1 is now replaced by e to the alpha t times H1. So, now time appears here, here and also here it appears at three places. Over here it appeared only at two places okay. (Refer Slide Time: 44:00)

$$H_I = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iH_0 t}{\hbar}}$$

The following two results remain valid under adiabatic switching when $H_1 \rightarrow (e^{\alpha t} H_1)$

(1) $i\hbar \frac{\partial}{\partial t} U(t, t_0) = H_I(t) U(t, t_0)$

(2)

$$U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

PCD STITACS Unit 4 Feynman Diagram Methods 48

This is the relation that we developed, the differential equation for the time evolution operator and the integral solution okay. Now this is going to remain valid even if H_1 goes to $e^{\alpha t} H_1$ okay there is no reason why this would change. So, one can do the same thing and show it explicitly.

But nothing in what we have done you know comes another way of using this. So we and we are going to use the both of these results with the difference that H_I is now made up not just of this H_1 but H_1 times $e^{\alpha t}$. So, that is the difference that we are now going to incorporate in the rest of the analysis.
 (Refer Slide Time: 44:46)

$$H_I = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iH_0 t}{\hbar}}$$

$$\Omega_I = e^{\frac{iH_0 t}{\hbar}} \Omega_S e^{-\frac{iH_0 t}{\hbar}}$$

Interaction picture

$$\psi_I(t) = U(t, t_0) \psi_I(t_0)$$

$$\psi_S(\vec{r}, t) = e^{\frac{iH_0 t}{\hbar}} \psi_S(\vec{r}, t)$$

picture

$$H_I(t) U(t, t_0) = i\hbar \frac{\partial}{\partial t} U(t, t_0)$$

The time development operator must explicitly depend on α

$$H = H_0 + H_1 \quad \psi_I(t) = U_{\alpha}(t, t_0) \psi_I(t_0)$$

$$U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

$$U_{\alpha}(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

PCD STITACS Unit 4 Feynman Diagram Methods 49

So, here we are, we have got the interaction picture operators and state functions. You have got the interaction picture operator corresponding to the perturbation part or the correlation part or the part which is the unfriendly part as I sometimes call it okay. But the time

development operator now in some sense must explicitly respect the fact that we have inserted a mathematical artificial term.

Because I could use an alpha which is the tiny small number and you could use a different alpha may be a beta which is also a tiny small number right but different from what I had chosen okay. So, whichever is being used must be kept track off and therefore I put a subscript alpha on this U and I write this Psi i t has U subscript alpha t, t0 Psi t0.

So, this alpha is going to keep track of the fact that some particular choice has been made whatever although in the limit at the end and what you started out with will not matter after you have taken the limit alpha going to 0. But not until then so at this point we have not taken the limit alpha going to 0 and we must therefore keep track of what alpha was chosen, so this time evolution operator.

Now will be written with a subscript alpha to remind us that a particular switch adiabatic mathematical switch alpha has been used, so now this is the general solution that we had written earlier and we write it on in an equivalent form but respecting the choice alpha where the full Hamiltonian is no longer H0 + H1 rather it is H0 + H1 times e to the alpha t. So, it is the same solution but now you have got the subscript alpha okay.
(Refer Slide Time: 47:13)

$$H_t = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t H_1}) e^{-\frac{iH_0 t}{\hbar}}$$

Two limits that concern us
 $t \rightarrow -\infty$ and $\alpha \rightarrow 0$

as $t \rightarrow -\infty$; $e^{\alpha t} \rightarrow 0$ & $H = H_0 \leftrightarrow$ soluble part

$$H_0 \Phi_0 = E_0 \Phi_0$$

$$\Phi_0 : \text{time-independent stationary eigenstate of } H_0$$

Time evolution of the Schrodinger state if there were no 'correlations'

$$\psi_S(\vec{r}, t) = e^{-\frac{iH t}{\hbar}} \psi(\vec{r}, 0) \stackrel{H \rightarrow H_0}{=} e^{-\frac{iH_0 t}{\hbar}} \Phi_0(\vec{r})$$

NPTEL
 PCD STITACS Unit 4 Feynman Diagram Methods
 50

So, let us take it further now and we are in particular interested in two limits t going to minus infinity when we know what the solution is that is the soluble part of the Hamiltonian the other limit which is important to us is the limit in which we are really interested alpha going to 0. So, we have discussed what happens when t goes to minus infinity you get the soluble part right.

And the soluble part is this $H_0 \Phi_0 = E_0 \Phi_0$ this is the solid Schrodinger equation you know the exact solution. This is the time independent stationary Eigen state of the unperturbed Hamiltonian the H_0 the solvable part of the Hamiltonian and how does this Schrodinger state evolve with time it evolves as $e^{-i H t / \hbar}$ this is the time evolution operator right.

And as t goes to minus infinity your Hamiltonian is actually H_0 right. In the interaction picture you have got the full Hamiltonian over here. But this full Hamiltonian in the limit t going to minus infinity is H_0 . So, you have got $e^{-i H_0 t / \hbar}$, so instead of this H you can write H_0 over here okay.

(Refer Slide Time: 48:48)

$|\psi_i(\vec{r}, t = -\infty)\rangle = |\Phi_0\rangle$

$H = (H_0 + e^{i\alpha t} H_1)$

$H_{t \rightarrow -\infty} \rightarrow H_0$

$|\psi_i(\vec{r}, t=0)\rangle = |\Psi_0\rangle$
 $= U_\alpha(t=0, t=-\infty) |\psi_i(\vec{r}, t=-\infty)\rangle$
 $= U_\alpha(t=0, t=-\infty) |\Phi_0\rangle$

Two limits that concerned us: $t \rightarrow -\infty$ & $\alpha \rightarrow 0$

Next class:
 What happens in the limit $\alpha \rightarrow 0$?

Gell-Mann and Low theorem

Bye!

NPTEL

PCD STITACS Unit 4 Feynman Diagram Methods

Questions: pcd@physics.iitm.ac.ic 55

So, that is what we have got over here and now we ask this is how the Schrodinger picture wave function evolves with time. We ask how the corresponding interaction picture wave function involving time would and we know the answer the interaction picture wave function would evolve has this.

As the Schrodinger picture wave function operated upon by $e^{-i H_0 t / \hbar}$ this is the soluble part of the Hamiltonian. And what it essentially means is that these two are exactly equal when $t = 0$, it becomes independent of time, it becomes completely independent of time and just like the Heisenberg picture wave function right.

In the Schrodinger picture it is the wave functions which depend on time, the operators do not. In the Heisenberg picture it is the other way around right. So that is what we have got here. We will discuss now the limit α going to 0 because there are these two limits which are of interest to us t going to minus infinity we discussed that.

The other limit which is of interest to us is α going to 0 and when we do that we get a very important result in quantum field theory which is known as the Gell-Mann and Low theorem okay. So, we will discuss this in our next class there is any question today I will be happy to take, if not goodbye for now and then we will meet in the next class.