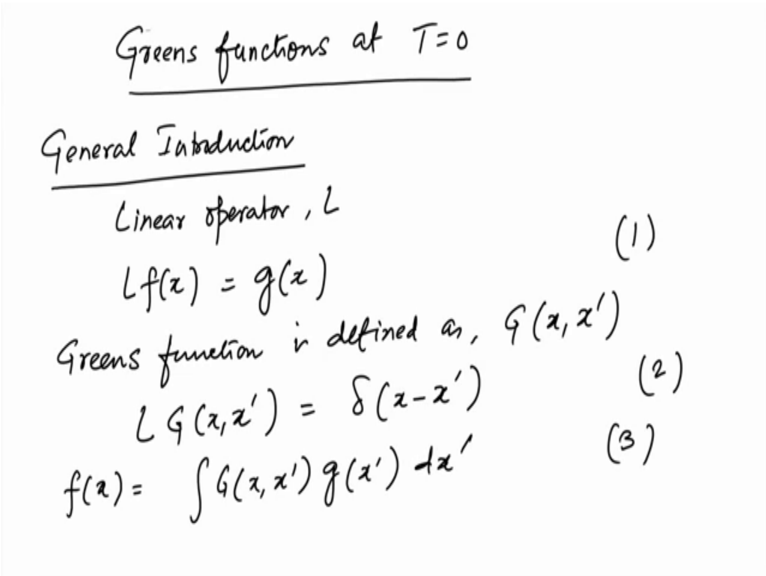
Advanced Condensed Matter Physics
Prof. Saurabh Basu
Department of Physics
Indian Institute of Technology, Guwahati

Lecture – 10
Green's function and representations in quantum mechanics

So, we shall talk about greens functions and in particular we will start with Green's functions at 0 temperature.

(Refer Slide Time: 00:31)



So, T equal to 0 and then we will learn how to extend it to finite temperature, but before we go on to discuss Greens function at T equal to 0 we will have do a number of things and the thing that we want to start with is a basic definition of greens function. Now if you remember that we have introduced greens function in the context of propagators and the retarded propagator was identified as Greens function and also the advanced propagator was introduced in that context.

So, I will give brief introduction to what Greens functions are and how they are relevant to condensed matter of physics or many body phenomenon in condensed matter physics. So, general introduction is what we plan to start with and this is slightly mathematical in nature in the sense that definition is mathematical in nature, but you will find that what we get at the end of it is quite useful in the context condensed matter physics. So, let us have a linear operator L which when operates on a function f of x it heals a g of x. So, this is a linear operator and f x is any arbitrary function which is a function of one variable and it gives a g of x.

And the Greens function is defined as so, we write greens function by G x, x prime where the L the same linear operator operating on G x, x prime gives me a derived delta function which is delta x minus x prime. Now let us say this is equation 1 and this is equation 2. So, one can write down the solution of a equation 1 in terms of the greens function as so, f of x is equal to G of x, x prime and g x prime d x prime. So, the solution of 1 is given by 3 which invokes the greens function. Now this is the general definition of mathematical definition of greens function, we have to understand that how it is of relevance to the study that we are presently involved in and for that.

(Refer Slide Time: 03:46)

Schrödinger Equation,

$$H|\psi(t)\rangle = i\hbar \frac{\partial|\psi(t)\rangle}{\partial t}$$

$$|\psi(x,t)\rangle = \int dx'\, G(x,x';t)\, \psi(x',0)$$

Where $G(x,x';t) = \langle x| e^{-iHt/\hbar} |x'\rangle$

Completeness relation,

$$\int dx'\, |x'\rangle\langle x'| = \mathbb{1}$$

Green operator, $G(t) := -i\,\Theta(t)\, e^{-iHt/\hbar}$

$\Theta(t)$ is the Heaviside step function.

Let us take this Schrodinger equation and this is equal to H acting on a wave function psi t this is equal to del psi del t that is the definition of that is the Schrodinger equation that we are all familiar with and the solution of this is given by psi of t in terms of the greens function as d x. So, this is a in principle of function of both x and t and so, we will write it with x and t and this is a d x and as a G x, x prime t psi x, 0.

So, this is the integral solution of the differential equation that we have written above which is Schrodinger equation and the psi the wave function at any given space time point can be generated from psi x 0 or rather this is x prime 0 by taking contribution from all x prime points and introducing the greens function here. So, where the G x, x prime t is equal to exponential minus i H t over h cross and a x prime and this is very easy to see, but this comes from the completeness relation of the wave functions that is d x prime the outer product of this should be equal to 1.

So, this is the, this is how the wave function at a given space time point can be calculated starting from a psi of x 0 here we are written x prime as a dummy variable and all x primes are being summed over we have introduced this concept earlier. So, I will skip here and go on to define Green operator which is defined as G of t and it is with the minus i and a theta function and exponential minus i H t by H cross. So, just to remind you, this theta function takes a value 1 when t is greater than 0 and it takes a value 0 when t is less than 0. So, theta t is the usual Heaviside function Heaviside step function. So, let us go to the Fourier transform of this green operator.

(Refer Slide Time: 07:24)

Fourier transform of the Green operator,

$$G(\varepsilon) = \int dt\, G(t)\, e^{i\varepsilon t/\hbar} = -i\int dt\, \Theta(t)\, e^{it(\varepsilon-H)/\hbar}$$

$$\Theta(t) = \frac{1}{2\pi i}\int d\omega\, \frac{e^{-i\omega t}}{\omega - i\eta}$$ η : infinitesimal parameter.

Recognize, $\delta(\omega) = \frac{1}{2\pi}\int dt\, e^{i\omega t}$

$$G(\varepsilon) = -\int d\omega\, \frac{1}{\omega - i\eta}\,\delta(\omega + \varepsilon - H)$$

$$= \frac{1}{\varepsilon + i\eta - H}$$

Energy spectrum is the pole of the Green's function.

So, the Fourier transform of the green operator is G of epsilon which is a canonical variable which is energy, which is canonical to the time and this is equal to d t G of t exponential i epsilon t by h cross. Now, this can be written as minus i d t and the definition of G there and this is equal to i t minus H by h cross. So, this is the Fourier transformed green operator and also we can write down theta function the integral representation of the theta function which is equal to 1 by 2 pi i and the d womega exponential minus i womega t divided by womega minus i eta. So, this is the it can be easily shown by doing a contour integration that this is equal to this the right hand side is equal to 1 when t is greater than 0 and x equal to 0 when t is less than 0.

Now, eta is an infinitesimal parameter and so, one can check easily by direct integration and now recognize that there is another form of the derived delta function where delta of womega is written as 1 over 2 pi and the d t exponential i womega t. And so, G of epsilon can simply be written as minus d womega 1 by womega minus i eta delta function of womega plus epsilon minus H and this gives me when integral of this is epsilon minus plus i eta minus H. This establishes a very important relation from the point of view of condensed matter physics that for a given system if we know what G of epsilon is or G of womega is, if you wish to write it that way then it gives you the energy spectrum as a pole of the greens function.

So, energy spectrum is the pole of the greens function so, this is the basic introduction to the greens function now we will get ahead with this form or rather the discussion of the greens function, but before that we wish to say that greens function will be written in representation which is called as the interaction representation. So, there are 3 kinds of representation that are used in quantum mechanics and so, they are called as Schrodinger representation, Heisenberg representation and interaction representation and their silent features are discussed.

(Refer Slide Time: 11:33)

$$i\hbar \frac{\partial \psi(t)}{\partial t} = H\psi(t) \Rightarrow \psi(t) = e^{-iEt/\hbar}\psi(0) \rightarrow S$$

$$\left.\begin{aligned} O(t) &= e^{iHt/\hbar}\, O(0)\, e^{-iHt/\hbar} \\ i\hbar \frac{d\hat{O}(t)}{dt} &= [O(t), H] \end{aligned}\right\} H$$

Expectation values,

$$\left.\begin{aligned} &\langle \psi_1(t)|O(0)|\psi_2(t)\rangle \\ &= \langle \psi_1(0)|e^{iHt/\hbar}\, O(0)\, e^{-iHt/\hbar}|\psi_2(0)\rangle \end{aligned}\right\} S$$

$$\left.\begin{aligned} &\langle \psi_1(0)|O(t)|\psi_2(0)\rangle \\ &= \langle \psi_1(0)|e^{iHt/\hbar}\, O(0)\, e^{-iHt/\hbar}|\psi_2(0)\rangle \end{aligned}\right\} H$$

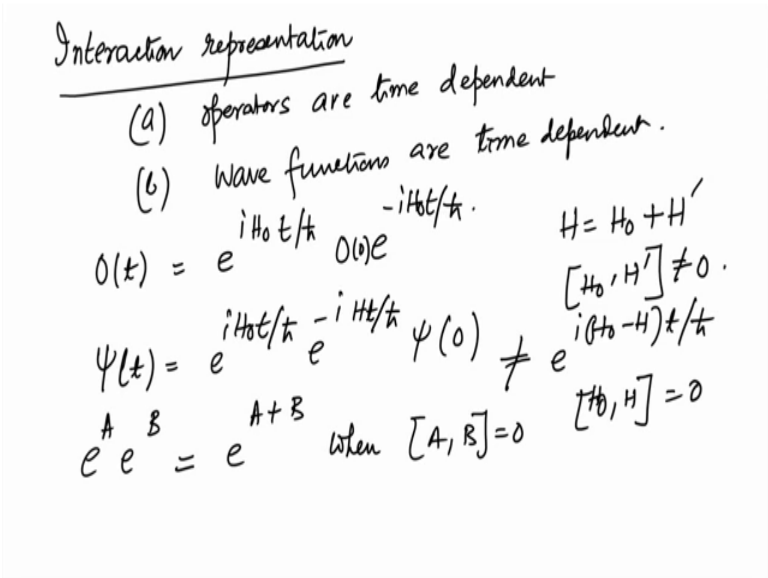
So, one is the Schrodinger representation and the Schrodinger representation is where the wave function is time dependent and the operators are all time independent. So, to distinguish it strong the Heisenberg representation and where the wave functions are time independent and operators are time dependent. So, let us take this discussion a little farther and let us write down in the Schrodinger representation so, will call it as s for the Schrodinger representation. So, in S representation we have the Schrodinger equation is equal to H psi t H is independent time and psi carries the time dependence and psi of t is given by trivial face factor which is minus i E t by h cross psi of 0.

So, now, this is in S representation and in H representation we have in the H representation we have operator any operator which could be the Hamiltonian in this case is given by exponential i H t by h cross 0 exponential minus i H t by h cross where H is the Hamiltonian and the equation of the motion for the operator is given by d d t or t del t which is equal to O t and H. So, this is the let us write it a little neatly and this is equal to so, this is the equation of the motion and these are in the Heisenberg picture. Now whichever picture you take the expectation values of the operators there should be independent of the representation. So, keeping that in mind let us take an operator o and calculate it is expectation values between 2 operator between 2 states. So, that is given by psi 1 and psi 2 in the Schrodinger representation.

So, this can be written as so, this is in S this can be written as psi 1 0 exponential i H t over h cross O at o is an independent O is a operator which is independent of time and this is exponential minus I H t by h cross psi 2 0 and this is in the Schrodinger representation and similarly in the Heisenberg representation my wave functions are independent of time and the time dependence is carried by the operators and then this can still be written as just the same by using the relation a for the operator the time dependence of the operator in terms of the Hamiltonian.

So, this can be written as exponential i H t over h cross O c o exponential i H t over h cross psi 2 of 0. So, this is in the Heisenberg representation and you can see that both the representations off course give rise to the same expectation values which is what it should be because a expectation values are physical observable sorry physical quantity we should not depend on the representation in quantum mechanics that you are considering.

(Refer Slide Time: 17:35)



So, then the interaction representation is where the both. So, operators are time dependent and wave functions are time dependent as well. So, the operators have a time dependence which is given by O t which O is an operator and this is i H naught t over h cross and O e minus i H naught t by h cross, where it is assumed that the total Hamiltonian it is written as a non interacting part which is H 0 and there is an interaction part which is H prime. So, the operator the time evolution of the operator only involves the non interacting part of the Hamiltonian and farther it is assumed that H 0 does not commute with H.

So, the wave function has a time evolution which is given by exponential i H naught t by h cross exponential minus i H t by h cross psi of 0 now remember that you cannot write it as exponential i H naught minus H t over h cross because this is possible only when H naught and H commute since they do not commute you cannot write it as combining the exponentials and you have to keep both of these things separately. So, basically what I mean is that exponential A, exponential B where both A and B are operator, if we exponentiate them is only equal to exponential A plus B and when A and B operators commute if they do not commute then you cannot write it that is why you cannot combine the exponentials.

(Refer Slide Time: 20:30)

Expectation values

$$\langle \psi_1(t) | \hat{O}(t) | \psi_2(t) \rangle = \langle \psi_1(0) | e^{iHt/\hbar} e^{-iH_0 t/\hbar} \left(e^{iH_0 t/\hbar} O(0) e^{-iH_0 t/\hbar} \right) e^{iH_0 t/\hbar} e^{-iHt/\hbar} | \psi_2(0) \rangle$$

$$= \langle \psi_1(0) | e^{iHt/\hbar} O(0) e^{-iHt/\hbar} | \psi_2(0) \rangle$$

Let us just check the expectation values of the operators in this representation. So, expectations values and this is psi 1 t o t psi 2 t is the expectation value of the operator o in the between the states psi 1 t and psi 2 t and this can be written as psi 1 0 exponential i H t by h cross exponential minus i H naught t by h cross and for the for the operator it has to be written as exponential i H naught t by h cross o 0 exponential minus i H naught t by h cross and then the other term has to be written that site which is equal to exponential i e H naught t by h cross exponential minus i H t by this and there is a psi 2 0.

So, if you look at this then these cancel and as well this and this cancel giving me exactly the thing that, I we want that is psi 1 0 exponential i H t by h cross o 0 and exponential minus i H t by h cross and psi 2 0. So, it is clear that the expectation values are independent of any representation that you take and it is been shown to be the same in Schrodinger, Heisenberg and interaction representation. So, will just tell you in while that why these representation are being introduced and the utilities of that, now let us show that how the time dependence of the wave function is governed by the interaction term H prime.

(Refer Slide Time: 22:58)

$$H = H_0 + H' \qquad \psi(t) = e^{iH_0t/\hbar} e^{-iHt/\hbar}\psi(0)$$

$$\frac{\partial}{\partial t}|\psi(t)\rangle = i e\, e^{iH_0t/\hbar}(H_0 - H)\, e^{-iHt/\hbar}\psi(0)$$

$$= -i e\, e^{iH_0t/\hbar} H' e^{-iHt/\hbar}\psi(0)$$

$$= -i\, e^{iH_0t/\hbar} H' e^{-iHt/\hbar}\left(e^{iH_0t/\hbar} e^{-iH_0t/\hbar}\psi(0)\right)$$

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -i H'(t)\psi(t)$$

Let us introduce an operator,

$$U(t) = e^{iH_0t/\hbar} e^{-iHt/\hbar} \quad \text{with } U(0) = 1$$

EOM for U, $\frac{\partial}{\partial t}U(t) = -ie\, e^{iH_0t/\hbar}(H_0 - H)\, e^{-iHt/\hbar}$

So, once again just remind you that my H is written as H 0 plus H prime where H naught is the non interacting Hamiltonian part of the Hamiltonian and H prime is the interaction part. So, let us see that how the wave function the time dependence of the wave function is related to the H prime. So, this is equal to i e exponential i e H naught t by h cross H naught minus H exponential minus i H t by h cross psi of 0. This we have taken the definition of psi reference just while back to remind you that that while put the definition once again here.

So, psi t is equal to exponential i H naught t by h cross exponential minus i H t by h cross and psi of 0. So, once you have to keep the first term constant and take a derivative of the second term and then again you have to keep the second term constant and take the derivative of the first term and this is what comes after that and so, H naught minus H is equal to minus H prime. So, this is equal to minus i e exponential i H naught t by h cross and H prime exponential minus i H t by h cross psi of 0 and I can simply introduce a exponential i H naught t.

Here become exponential minus i H naught t. So, that is minus i exponential i H naught t by h cross H prime exponential minus i H naught t by h cross and now in a bracket I would like to introduce this which is nothing, but introducing a one there and psi of 0. So, this will be this can be written as. So, this is so, delta t of psi t is nothing, but equal to this is nothing, but equal to minus i H prime t and psi of t we have just used the definition of psi of t here and writing it as. So, this exponential i so, there is this term which is which gives me H prime and. So, these things will combine to give me these time derivative or time evolution of the wave function.

So, this is the equation of the motion for the wave function which involves H prime you can fill in line here or step here and let us introduce an operator which is U of t, which is equal to exponential i H naught t by h cross exponential minus i H t by h cross with U 0 U at t equal to 0 is 1. So, the equation of the motion for U I am writing it short hand. So, equation of motion is e o m for U is del del t of U t again I am going to take derivative with respect to time meaning that first one will kept constant and second one will be taken derivative and so, on.

So, then it becomes equal to exponential i H naught t by h cross and a H naught minus H exponential minus i H t by H cross. So, that is the equation of motion for U and if you look at the equation of motion for U and equation of motion for psi they look identical.

(Refer Slide Time: 28:07)

$$\frac{\partial}{\partial t} U(t) = -i H'(t) U(t).$$

EoM for $\psi(t)$ and $U(t)$ are identical.

$$U(t) = U(0) - i \int_0^t dt_1 \, H'(t_1) U(t_1)$$

$$U(t) = 1 - i \int_0^t dt_1 \, H'(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \, H'(t_1) H'(t_2) + \cdots\cdots$$

$$= \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, H'(t_1) H'(t_2) H'(t_3) \cdots H'(t_n).$$

So, this can also be written as del del t of U t which is equal to a minus i H prime of t and U of t. So, this is the equation of motion for U so, EOM for psi of t and U of t are identical. Now since that is correct then we can solve either of psi of t or U of t and can write down the solution for say U of t here equal to U 0 minus i minus it is 0 to t and a d t 1 H prime t 1 and a U of t 1. So, this is the solution of this equation that appears at the top of the page which is for the equation of motion for U. So, U has the solution has the time evolution which is given by this, but the only problem with this form is that both the left hand side and right hand side are they involved the same variable unknown variable which is U of t. So, if you repeat this procedure for the right hand side as well will get an iterative solution by doing it so, U of t 1.

We can write down again an integral expression of the kind that we have written for u of t and then again will get a U t 2 for which we can write down again repetitive solution, integral solution and will get a series which is like this. So, U of t is equal to now since U of 0 has taken to be equal to 1. So, we can write simply equal to 1 and 0 to t d t 1 H prime t 1 plus minus i square 0 to t d t 1 0 to t 1 d t 2 and H prime t 1 and a H prime t 2. So, this is the second term and there will be farther terms which finally, can be combined with n equal to 0 to infinity and you have a minus 1 whole to the power n and a 0 to t d t 1 and 0 to t 1 d t 2 and so, on and 0 to t n minus 1 d t n and we have so many of these interaction terms you just write them little neatly t 1 H prime t 1 H prime t 2 H prime t 3 and so, on all the way of to H prime t n.

So, this is the solution series solution of the, for the operator that we have introduced U of t and hence it should also be the solution for psi of t as we have seen that the psi of t and U of t have the same equation of the motion. Now it is important to introduce time ordering here and that is going to be quite helpful.

(Refer Slide Time: 32:02)

Introduce time ordering operator, T

$$T\left[H'(t_1)H'(t_2)H'(t_3)\right] = H'(t_3)H'(t_1)H'(t_2)$$

$$t_3 > t_1 > t_2$$

Step function is interesting in this Context,

$$\theta(x) = 1 \quad \text{for } x > 0$$
$$= 0 \quad \text{for } x < 0$$
$$= \frac{1}{2} \quad \text{for } x = 0$$

$$T\left[H'(t_1)H'(t_2)\right] = \theta(t_1-t_2)H'(t_1)H'(t_2) + \theta(t_2-t_1)H(t_2)H'(t_1)$$

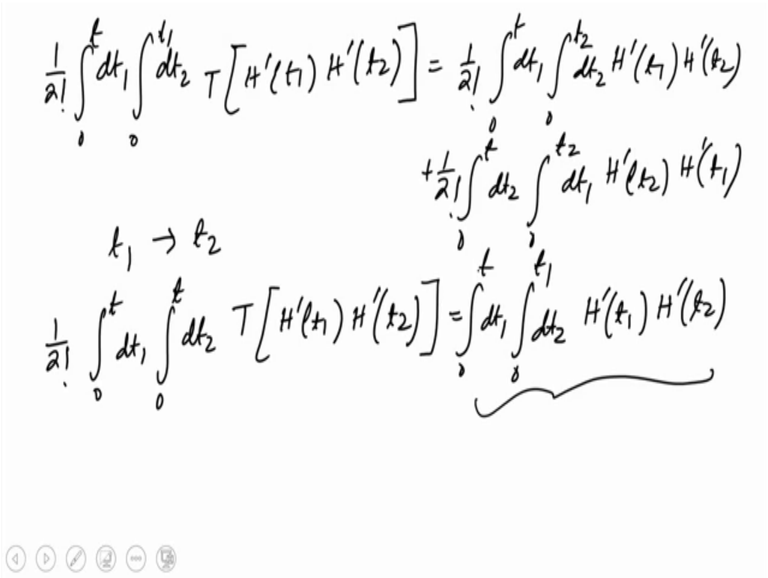
$$\left[H'(t_1), H'(t_2)\right] = 0 \Rightarrow \text{ordering is unimportant.}$$

So, introduce time ordering operator let us call it as t and what it does is that it does. So, H prime t 1 H prime t 2 and H prime t 3 and it just with the earliest time it puts us to the left. So, H prime t 3 H prime t 1 and H prime t 2 if t 3 is greater than t 1 is greater than t 2 so, that is what it does this is an important step which I think you should take a note of this that we have a time we have introduced the time ordering operator which acts on a series of interacting Hamiltonians written as a different times t 1 t 2 t 3 and it puts as you apply the time ordering operator it puts the Hamiltonian or the interaction part of the Hamiltonian with the earliest time that is the time which is greatest on the left and then orders it accordingly and then next one goes after that and the next one after and so, on this is the time ordering of operator.

So, a this also step function that we are using which is not exactly the hemiside step function, but it is something very similar to the that step function is interesting or rather is important here interesting in this context and this is theta of x equal to 1 for x greater than 0, x equal to 0 for x less than 0 x equal to half for x equal to 0. So, how the t is written so, it is take 2 times H prime. So, the time ordering operator operates on Hamiltonian at 2 distinct times and. So, there is a possibility that t is greater than t 1 is greater than t 2 which is the case for the first one and if not then the other possibility is given by t 2 minus t 1 H prime t 2 H prime t 1.

So, that you have taken into account both the possibilities which t 1 is greater than t 2 and t 2 is greater than t 1 if in a particular case if t 1 is greater than t 2 then only the first terms survive and the second term will be dropped to 0 and remember one thing that if H of t 1 H prime of t 1 and H prime of t 2 would have commuted and they commute then these ordering is unimportant, but since they do not the ordering becomes important. So, let us look at the time ordering operator a little more carefully.

(Refer Slide Time: 36:04)



So, let us just write 1 by 2 factorial which is nothing, but 1 by 2 which is a d t 1 I am just looking at a particular case where for 2 time variables t 1 and t 2. So, this is from 0 to t 1 and this is equal to time ordering of H prime t 1 and H prime t 2 which is equal to 1 by 2 factorial 0 to t d t 1 0 to t 1 d t 2 H prime t 1 H prime t 2 plus 1 by 2 factorial 0 to t d t 2 0 to t 2 d t 1 H prime t 2 and H prime t 1.

Now, if you see the first and the second terms they are identical under the swapping of t 1 to t 2 and visa versa this t 2 back to t 1, then we can write down that 1 by 2 factorial 0 to t d t 1 0 to t d t 2 time ordering of H prime t 1 H prime t 2 this is equal to 0 to t d t 1 and 0 to t 1 d t 2 H prime t 1 H prime t 2 and so on. So, you do not know that something like this had appeared in our solution for U of t and this we are able to write down as time ordering of 2 operators. So, many of n operators will have a 1 over n factorial and simply we can write down that term.

(Refer Slide Time: 38:21)

Example for 3 times t_1, t_2, t_3

$$\frac{1}{3!}\int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3 \, T\left[H'(t_1) H'(t_2) H'(t_3)\right]$$

$$= \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \, H'(t_1) H'(t_2) H'(t_3)$$

$$U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \, T\left[H'(t_1) H'(t_2) \cdots H'(t_n)\right]$$

$$= T \exp\left[-i \int_0^t dt_1 \, H'(t_1)\right]$$

Same solution is applicable to $\psi(t)$

So, we will just so, for 3 time ordering operator just give one more example, example for 3 time times t 1 t 2 and t 3 and this is equal to 1 by 3 factorial and this is 0 to t d t 1 0 to t 1 d t 2 and 0 to t 2 d t 2. So, what 1 is going to happen in is there is a 0 to t and there is a 0 to t. So, this has to be 0 to t all are 0 to t and we have. So, this is equal to a d t 3 and now I have a t H prime t 1 H prime t 2 and H prime t 3 and this is equal to a 0 to t d t 1 0 to t 1 d t 2 and 0 to t 2 d t 3 H prime t 1 H prime t 2 and H prime t 3. So, we really do not need to care about which time comes first or which time is the earlier time as compared to others.

So, we can simply write it with the time ordering operator and now also note that all the time integrals go from 0 to t and this time ordering takes care of everything. So, using this time ordering operator the solution of the operator that we had introduced is U of t can be written as 1 plus and there is a n equal to 1 to infinity and there is a minus 1 whole to the power n by n factorial and now you have a 0 to t sorry again. There is a 0 to t and d t 1 d t 1 and 0 to t d t 2 and all that and then 0 to t there is a d t n this and H prime t 1 H prime t 2 and the way up to H prime t n.

This is the complete solution of U of t and hence reminding you the hence it is also the complete solution of psi of t this because it is an infinite series because this n there is a sum goes from one to infinity we can write this as an exponential with the time ordering operator outside. So, it is t exponential minus i 0 to t and d t 1 and a H prime and t 1. So, that is the solution of U of t and and also. So, same solution persists or rather you should write is applicable to psi of t.

So, thus if we know the U of t then we can also know how psi of t evolves and for that we have to know the interaction term act different time intervals H t 1 t 2 etcetera. So, if for a given, so the idea is this that a particle is actually introduced into an interacting path and it undergoes a scattering with other particles sorry it is acted upon by an external interaction potential that is also possible and which.

So, it undergoes H prime at t 1 t 2 t 3 etcetera and this whole solution can be written as the time ordering operator multiplied by the exponential of this which involves the interaction term act given t 1 and has been integrated from 0 to t. So, this is the solution of psi of t and will see that how to one gets a Greens function from here.