## **Dynamics of Classical and Quantum Fields: An Introduction Prof. Girish S. Setlur Department of Physics Indian Institute of Technology, Guwahati**

# **Nonequilibrium Green functions Lecture - 43 S-Matrix Perturbation Theory**

Ok. So, let me continue where I left off. So, if you remember that I was trying to motivate the introduction of Nonequilibrium Green's function.

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So, the idea was that if the system was in equilibrium; that means, there was some kind of a reservoir at some temperature t n which is basically 1 by beta and the system was in thermal contact with the reservoir. So, it would come to an equilibrium and in such a situation I hopefully manage to convince you that the particle Green's function and the whole Green's function are related to each other in a rather simple way. If you pretend that the times that are involved are on the imaginary axis.

So, in other words if I shift one of the times to the original time minus i beta h bar I get back the if it is a particle Green's function I will get back the whole Green's function except that there will be some factor which is either positive or negative depending upon whether it is boson or fermion. So, bottom line is that there is this kind of a periodicity. So, in other words the particle Green's function becomes the whole Green's function and the whole becomes particle if I shift by a discreet amount on the imaginary axis.

And besides the Green's functions for systems in thermal equilibrium basically equilibrium Green's functions are time translation invariant; that means, if I shift my origin of; that means, if I call the 0 of my clock something else. So, I am measuring times using a clock. So, instead of calling 0 what it was earlier I call my 0 of the clock. I start counting from some other time nothing is going to change because you see the Green's function depends only on the time elapsed between the.

So, in equilibrium the Green's function will only depend on the time elapsed between inserting a particle and removing a particle if I am talking about say the particle Green's function, but it depends upon. So, if I am talking about the whole Green's function it would depend upon the time interval between removing a particle and inserting the particle.

So, bottom line is it only depends on the difference between the times the two times that are involved. So, similarly if the system is spatially homogeneous and that would be the case for example, if there are no external there is no positive charge that is you know located at some discrete lattice points. So, if there are positive charges located at discrete lattice points that is typical in a solid then of course, the Green's function will continue to be temporarily homogeneous.

That means that there will be time translation invariance, but the space translation invariance will not be there. Except there may be a discrete space translation invariance, but the continuous smooth type of translational invariance in space will be absent. But it is typical you know in many body theory to pretend. So, even if you are. So, you might be thinking that when is the situation you will encounter where you will encounter a spatially homogeneous system, because that seems rather unnatural in a solids.

Because in solid the positive charges are located at some fixed lattice location, so there is, so there the spatial homogeneity is lost. So, now the answer to that question is that you can still you know. So, if your goal is to study the many body dynamics of the electrons in the solid it is really a distracting complication to have a lattice to deal with. So, that means, it is better to somehow make the lattice less important because we are interested in highlighting the many body aspect of the problem.

So, the way to highlight the many body aspect of the problem is to introduce a device called the jellium. So, that means, the jellium is a kind of a fictitious caricature or a cartoon of a solid. So, there you take a real solid and you look at the positive charges which are located at those fixed points I mean at those lattice points. Then you retain those I mean in your this is all in your head I mean in your mind it is a mental picture.

So, you pretend those positive charges are something that you can smear out with your fingers. So, the strength of you see the positive charges you just think of them as pencil marks on a piece of paper. So, because all those positive charges are concentrated at a point that pencil mark will be very dark and very localized, because it is all concentrated at a point.

So, now imagine you place a finger on a pencil mark which corresponds to a positive charge at a lattice point. And then you just rub your finger around and smear out that positive charge all over the inter particle spacing; that means, the inter atomic spacing will be white because it does not contain positive charges. So, you smear it out and you do it for all the other positive charges.

So, then you see you will be conserving the total positive charge because you are not destroying any charge because you are merely smearing it out. Now the plus point of doing that is now your positive charge is spatially homogenous because you have smeared it out. So, now, but then you see the even though you have smeared out the positive charges they still are inert. In the sense that the their only role is to provide charge neutrality. Because you see the actual system that we are dealing with that contributes to the dynamics is the electrons in the solid.

So, is the electrons in the solid that participate in the quantum dynamics. So, the positive charges are there just to hold the electrons together because otherwise without the positive charges the electrons being mutually, they are all negative charges. So, they will mutually repel and fly apart. So, there has to be something holding them together and that something holding them together should be only for that purpose.

Means its only job should be to hold the electrons together, it should not contribute to its own dynamics. I mean in a real solid it does, but then this is the cartoon version of the solid where I am trying to minimize these distracting complications and focus only on the many body aspects of the electrons. So, in that case I create this kind of a mental picture of a solid where the positive charges have all been smeared out and made uniform. And that uniform positive charge is completely inert and its only role is to provide charge neutrality.

And now the real objects or entities that participate in the quantum dynamics are the electrons. So, this sort of model of a solid cartoon model of a solid is called a jellium, ok. So, it is called jellium model jellium. So, it is quite popular and people study it, ok. So, but that was you know I mean I am just trying to remind you where I left off in last few classes. So, I was basically studying such a solid or even a solid with an actual lattice, but at equilibrium. So, the point is that the system is in contact with some surroundings.

So, but then in many other applications you may be interested in you know disturbing the system in question momentarily. Say maybe you want to shine a laser pulse on the system and try to you know use some very short time probes like femtosecond laser spectroscopy and try to find the dynamics of the electrons that you know how the electrons respond to such a short, but intense laser pulse.

So, in order to answer such questions which are of quite a significant importance and interest nowadays. Because technologically it is possible to you know achieve those kinds of high intensity very short laser beams that can probe you know processes that occur at picosecond sub picosecond time scales. So, in other words in order to do that you really have to understand how to generalize this concept of Green's function to systems that are now no longer in equilibrium.

So, when the system is not in equilibrium you can see that the Green's function is not a function anymore of the time difference between the two times. So, now, you see this external short duration disturbance determines in some sense it biases your origin of time selection; that means, it. So, because that disturbance happens at a given time. So, you it is more convenient to refer to time duration as being you know after this disturbance or before this disturbance.

So, now you see the system is no longer going to depend only on the time duration between creating and annihilating, but rather it also depends on how long after this disturbance you are doing that creating and annihilating. So, it is going to independently depend on those two times. So, that is the reason why you need a nonequilibrium Green's function.

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So, anyway I think I kind of these sort of qualitative descriptions are important. Because firstly, you know this formal algebraic manipulations and these formal proofs and all that in any case you can read them from the books and it is very it is not that convenient for me to describe in words what is going on. Because it is pretty self-evident what is going on you just need the patient to read whatever is written in the book. But nevertheless, I do not want to disappoint those of you who are actually interested in knowing from an instructor what is there in the books.

So, bottom line is I remember this is where I had stopped. So, I told you that in you know Heisenberg picture the annihilation operator evolves according to this. And so,

now, you see in a situation where the system is you know a system is such that the Hamiltonian is explicitly time dependent then you will be forced to introduce this evolution operator which depends on these two times, ok. So, it is going to depend on these two times and this is the so-called S matrix that depends on the part of the Hamiltonian that is explicitly time dependent.

So, after this it is a whole bunch of formal results. So, I am going to skip all this and tell you what it is I have achieved here. See bottom line is that whatever before this 10.90 and after 10.78.

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So, you might be wondering what are all these equations. Say basically those equations are merely required those steps are merely required to prove this sort of group property of this S matrix. So, it is like you know this is somewhat reminiscent of group theory. So, you have this S matrix and you compose it with some other matrix you will get some other.

So, it is something like a you can think of it in various ways, but bottom line is this is what it is. So, I have spent some few steps trying to prove this and then I have also proved that S is unitary. So, f dagger S is 1. So, these two put together are quite important because they will you know enable you to do many things nicely. So, now, the,

ok, so this is all rather straight forward algebra there is no physics content there. So, the real physics content comes in fact, will come a little later.



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So, in order to motivate the physics content, I have to tell you why we introduce this S matrix approach by the way is called the interaction picture. So, you remember that in quantum mechanics that three types of so-called pictures one is the Schrodinger picture where the operators are explicitly time independent, but the states the wave function or the states are time dependent. So, there is the exact opposite where the states are time independent, but the operators are explicitly time dependent.

So, that is what this would be for example, ok. So, 10.76 would correspond to the Heisenberg picture. So, the interaction picture is somewhere in midway between the Heisenberg and the Schrodinger picture. So, that means, what we do is that we say that both states and operators evolve with time except the state evolves according to the time independent part of the Hamiltonian, right. Whereas, the operators evolve according to the time dependent part of the Hamiltonian, so which is why there is this thing.

So, the idea is that the. So, this is the this is evolved according to 2 H. So, remember H of S is equal to h plus V of S. So, it is the V of S which is time dependent. So, this is time independent H is time independent. So, this operator is sitting in the middle with that carrot on top this hat or whatever you want to call it. So, that is evolving according to the time independent part of the Hamiltonian whereas, the this is the overall time evolution of the annihilation operator with respect to the full Hamiltonian.

So, now that full evolution is completely determined by this evolution with respect to the time independent part sandwiched between the S matrices. So, that is basically it.

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 $S(t,t_r)=T\left(e^{-\frac{i}{\hbar}\int_{t_r}^t\hat{V}(s)\ ds}\right),\qquad \wedge$  $(10.82)$ since  $S(t_r,t_r) \equiv 1$ . Going back to Eq. (10.76), we get,  $\psi(\mathbf{x},t)=S^{\dagger}(t,t_r)e^{i\frac{(t-t_r)}{\hbar}H}\psi(\mathbf{x},t_r)e^{-i\frac{(t-t_r)}{\hbar}H}\,S(t,t_r)$  $= S^{\dagger}(t,t_r) \hat{\Psi}({\bf x},t) S(t,t_r),$  $(10.83)$ where  $\hat{\mathbf{\Psi}}(\mathbf{x},t)=e^{i\frac{(t-t_r)}{\hbar}H}\mathbf{\Psi}(\mathbf{x},t_r)e^{-i\frac{(t-t_r)}{\hbar}H}.$  $(10.84)$ In general,  $S(t,t^{'}) = T\left(e^{-\frac{i}{\hbar}\int_{t^{'}}^{t}\hat{V}(s)\,ds}\right).$  $(10.85)$ Clearly,  $S(t,t) = 1$ . The above function obeys the equation of motion  $i\hbar \frac{\partial}{\partial t} S(t,t^{'}) = \hat{V}(t) S(t,t^{'})$  $(10.86)$  $i\hbar \frac{\partial}{\partial t'} S(t,t') = -S(t,t') \hat{V}(t'),$  $(10.87)$ and its Hermitian conjugate obeys  $-i\hbar\frac{\partial}{\partial t}S^{\dagger}(t,t^{'})=S^{\dagger}(t,t^{'})\hat{V}(t).$  $(10.88)$ This is unitary  $S^{\dagger}(t,t')S(t,t') = 1$ . To prove this, we first show that  $S^{\dagger}(t,t')S(t,t')$  independent of t by differentiating with respect to t. Then we choose  $t = t'$  since it is independent of t and the result follows.  $i\hbar \frac{\partial}{\partial x} (S^{\dagger}(t,t^{'})) S(t,t^{'}))$  $= (S^{\dagger}(t,t^{'}))\dot{t}\hbar \frac{\partial}{\partial t}S(t,t^{'})) + (\dot{t}\hbar \frac{\partial}{\partial t}S^{\dagger}(t,t^{'})S(t,t^{'}))$  $=(\boldsymbol{S}^{\dagger}(t,\boldsymbol{t}')\hat{\boldsymbol{V}}(t)\;\boldsymbol{S}(t,\boldsymbol{t}'))-(\boldsymbol{S}^{\dagger}(t,\boldsymbol{t}')\;\hat{\boldsymbol{V}}(t)\boldsymbol{S}(t,\boldsymbol{t}'))=0$  $(10.89)$ 

So, now why do we do this? Why do we introduce the S matrix? We introduce the S matrix because. So, remember if you want to think of this time dependent part as a perturbation. So, that means, if you want to think of this V as a perturbation what you have to do is it is very logical and very obvious that its convenient this S matrix approach is especially convenient to perform perturbation series. Because after all what is S? S is just the time ordering of this sort of an exponential in. Now if I expand in powers of V, I will just get a series.

So, basically that is what it is. So, now, so that is basically the motivation for introducing S matrix first of all. It is motivated because you are you can do perturbation theory cleanly. Because you see the thing the operators that are in between they are evolving according to the unperturbed part of the Hamiltonian which is also time independent. So,

the time dependent parts are the ones which are containing the S matrix in which you can nicely expand in powers of V.

So, but then, so that is the advantage of doing that. So, when you actually start performing this calculation you will then start to notice some not so convenient feature. And that not so convenient feature is already obvious here in 10.83. So, the not so convenient feature is the following that you see. So, you have committed to expanding in powers of this V of V which is the time dependent part of the potential, but then now we are forced to expand you are forced to perform this expansion in two places one is here and the other is here.

So; that means, you are forced to expand in powers of V in two different places. And that is not very convenient because then you will get all kinds of cross terms from all over if you go to high orders, you will get a bunch of cross terms which is really annoying and they are on either side of this psi. So, there is a very clever way of getting around this issue.

So, you might think that why should you get around this issue. So, be it I mean that if that is how it is, that is how it is. Let us just grin and bear it I mean the you might take that point of view. And technically you would not be wrong. I mean you know if you are willing to put in the effort nobody is going to prevent you, but then it is certainly not elegant especially in hindsight when you know that there is a better way.

So, the point is that there is a better way and that better way involves again you might have guessed that basically it involves the use of time ordering. So, the idea is that you cleverly define a notion of time ordering in such a way that now this S matrix no longer appears on either side of psi it only appears on one side of psi, ok. So, if it appears only on one side then it is extremely convenient because you just have to expand that one S which is sitting on one side.

And you simply go ahead and expand that. So, that is what I am going to try and convince you that it is possible at this stage it is not at all obvious it seems rather impossible. But the reason why it is possible is because you have to be a little clever; that means, you have to introduce the notion of time ordering in such a way that you can achieve this. So, now, what is that notion of time ordering? So, that is the reason why I have to improve this lemma.

So, you will have to bear with me. So, things are rather technical now I mean, but I have to motivate all this technical development and I have just told you what that is.

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So, the idea is that you see if you have operator psi which is the annihilation. So, I forgot a dagger there is a dagger there, ok. So, this is a misprint it should be a dagger psi it is not psi psi; psi psi dagger. So, you see there is this annihilation operator which is annihilating a particle at x at time t and then psi dagger is creating a particle at x dash t dash. So, now, the idea is that I am going to prove to you that there is.

So, I am going to prove this identity. So, basically the claim is that. So, you can always write the time ordered part of psi psi dagger this way the full psi psi dagger. So, this is a time evolution with respect to the complete Hamiltonian. So, now this can be rewritten in terms of the time evolution with respect to the unperturbed part of the Hamiltonian multiplied by these two S matrices. So, you might think that I still have not made one S matrix still two S matrix is on either side. So, you will have to be patient.

So, this is an intermediate step in that eventual goal where I am going to put all the S matrices on one side. Right now it is still on both sides here. But nevertheless, I have to prove this in order to achieve that final goal. So, the claim is that the time ordering of psi x comma t times psi dagger x dash t dash is given by an S matrix of this type. So, remember I have defined what that S t that t dash is. So, you go from minus to plus infinity and then the time ordering from here then back from plus to minus infinity. So, remember that this S matrix is inside the time ordering this is outside.

So, how do you prove this? I mean it is just quite straight forward all you have to do is you assume one case t is greater than t dash, right. So, and then you use this group property of this S matrix, ok. And then you start inserting and it is just straightforward I am not going to really go through all the steps. So, it is just you just keep inserting and then you will get your result, ok. So, it is pretty straight forward.

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And the proof for the other case is similar that if t is less than t dash also it is similar. So, therefore, ok. So, I am going to assume that you are all going to sit down and follow all these steps it is very irritating to explain this verbally, ok. So, you will have to sit down and do it yourself. So, now, assuming that you have understood that, then see therefore, the expectation value of this sort of time ordering of these two operators again if this is a miss print this is a dagger.

So, with respect to some state is clearly given by the expectation value with respect to the same operator, but now evolving according to the unperturbed Hamiltonian and sandwiched between these two S matrices, ok. So, now, it is still not very convenient still you have two S matrices and my goal of making sure that the S matrix appears only on one side of these operators is still elusive it has not been reached.

So, now the question is, how would you achieve that? Ok. So, the way is that I am going to make some assumptions, ok. So, the assumption is that this V of S is while it is time dependent it is adiabatic in the following sense; that means, adiabatic switching so; that means, what; that means, is that you imagine this external time dependent potential is 0 in the remote past and it is 0 in the remote future.

So; that means, it is switched on gradually in such a way that the state of the system so; that means, you imagine that in the remote past that the system had a well-defined energy suppose you decide because after all there is no question of temperatures this is a nonequilibrium problem. So, you can I mean it is not logically wrong to postulate that the system had a well-defined energy in the distant past.

So, if it has a well-defined energy in the distant past, I am going to assume that that energy is non degenerate; that means, there is exactly one state which corresponds to that energy. So, if that is the case then if I switch on a perturbation and I do it very slowly. So, there is a very good reason to expect that that state. So, if I switch it on slowly of course, it is going to finally, change, but then when I finally, gradually switch it off.

So, there is every reason to expect that the final state will basically be the same as the initial state So, the wave function of the final wave function and the initial wave function will correspond to the same state. So, that means, they differ only by a phase. So, you see the operator that takes the initial state to the final state is this one. So, it is the; it is the S matrix you evolve this S matrix from a distant past to the distant future. So, that is what this is doing. So, it is evolving the states from the distant past to the distant future, ok.

So, the claim is that this state, so this is the final. So, this is the initial state which is phi. So, it had a well-defined energy which is non degenerate and because it is non degenerate. So, it is like see if it was degenerate it is only a problem because what will happen is that the perturbation can actually create a superposition between these two states which have the same energy. So, the system kind of gets confused which state it is in because they all have the same energy.

So, if the perturbation will try to kind of you know jolt it into some superposition even though it was not in a super position earlier the perturbation can kind of suddenly reset that state into some super position if the state was degenerate, but we are not going to allow that. So, we are going to postulate that the initial state was non degenerate. So, if you slowly switch on and slowly switch off then having switched off you see the system is back in the original state. So, the worst that can happen is that two wave functions will differ by a phase. So, that is what is going to happen here.

So, you see there is this S matrix you are acting on the state and you get a phase. By the way I do not recall if I misspoke earlier. So, in interaction picture the operators change according to the unperturbed see that is what is happening here, right. So, the operators are evolving according to the unperturbed Hamiltonian whereas, the states are evolving according to the S matrix which is the perturbation. I might have said the reverse.

So, I do not recall now, but bottom line is this is what it is. So, this is the final state that is same as the initial state. So, therefore, they differ at worst by some kind of a complex number of unit modulus, ok.

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So, therefore, it is clear that its conjugate is this and it is this. So, that this e raise to i theta therefore, is trivially equal to the expectation value of the S matrix, ok. So, now, look at this part see, what is this? This is nothing, but it is e raise to minus i theta. And what is e raise to minus? So, its e raise to minus i theta phi, right. So, what is e raise to minus i theta it is 1 divided by this.

 So, which is basically, so e raise to minus i theta is basically 1 by expectation value of phi S infinity minus infinity phi. So, which is what this is means. So, what I have done is basically I have written this as 1 by this and now you see the numerator at least has only one S matrix. So, you might think that. So, what the denominator has another and you are back to square one. So, now, you still have two S matrices.

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Now, you see this interpretation is very convenient even though superficially there still remain two S matrices one in the numerator one in denominator. It is very convenient to do perturbation theory now because you see if you expand in powers of those. So, imagine lambda is imagine there is a lambda next to that V which is your time dependent perturbation. So, now, it is just a bookkeeping device which tells you how many V's are you are dealing with. So, lambda square means you are dealing with 2 V's. So, later on you can put lambda equal to 1 if you want.

So, bottom line is that you can expand this matrix in powers of this lambda and which just tells you how many V's you are dealing with. So, now, if you insert that expansion here in numerator and denominator you will see that and you expand the entire ratio in powers of lambda you will see that what it tells you is that you just have to deal. See when you are calculating this expectation value you just have to deal with the connected parts of this expectation value.

So, what; that means, is that when you are evaluating this throw away any term which looks like this; that means, throw away any term where the fields pair up with each other means that they kind of ignore everybody else and pair up amongst themselves. So, if they pair up amongst themselves you kind of disregard that. So, this is applicable to even two-point function.

So, this is one-point Green's function; that means, you are creating one I mean you are creating one particle destroying one particle. So, you can create two particles destroyed two particles. So, the same situation applies there also. So, the idea is that in any. So, when you are trying to evaluate this if you try to pair up you know you are forced to use.

Because you see remember that that is how you will be evaluating. You will be evaluating using something called Wicks theorem I do not recall if I explicitly explain to you what is Wick's theorem. So, Wick's theorem basically tells you that if you have a ok, that is not in general applicable. So, the bottom line is that basically it says that if in any calculation while trying to evaluate this you will be at some stage called upon to split it up into lower order moment.

So, this is a higher order moment this S 1 itself will contain psi dagger psi and so on. So, that is like the fourth four operators inside the expectation. So, typically you will try to reduce that to fewer operators. So, the point is that when you do that you will be pairing up various pairs like this a might be psi dagger psi sitting in S 1 like that. So, you will be pairing the psi here with some psi dagger sitting inside S 1 and so on.

So, the thing is that when you are doing that what this procedure says is that just do not include the pairing which involves pairing the original psi with the original psi daggers; that means, there were psi and psi dagger sitting there and do not include the pairing that involves pairing these two and just include. So, that those are those are the disconnected component because they are disconnected because they get disconnected. So, there is the original pairing is disconnected with the S matrix. So, they get separated out. So, do not include the disconnected pairing.

So, basically even though this S matrix still appears in both places this ratio still has the nice interpretation of only including the connected parts in the perturbation series. So, which is why we introduced this S matrix approach and this time especially this time ordering idea.

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So, this time ordering is explained nicely in this picture. So, I am going to. So, you can nicely combine various ideas in this way. So, so this is called the Keldysh contour, ok. So, this is called Keldysh contour. So, I am going to explain this may be in the next class. So, in the next class I will tell you more about what this Keldysh contour is and see where we can go from here.

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always larger in the C-loop sense than the latter. This allows us to take the S-matri<br>on the extreme left inside the time ordering to get,  $T_C(\psi(\mathbf{x},t)\psi(\mathbf{x}^{'},t^{'}))$  $=T(S_{C_-}(-\infty,\infty)S_{C_+}(\infty,-\infty)\ \hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}^{'},t^{'}))$  $\equiv T(S(C)\; \hat{\psi}(\mathbf{x},t) \hat{\psi}^{\dagger}(\mathbf{x}^{'},t^{'})).$  $(10.102)$ The S-matrix on the combined loop is  $S(C) \equiv S_{C_-}(-\infty, \infty) S_{C_+}(\infty, -\infty)$ , which is traversed in the clockwise direction. Typically, one is interested in weighted averages. For the purposes of the next section, we use the Search (e<sup>-B(H-pN)</sup>  $T(S(C) \hat{\psi}(x,t) \hat{\psi}^{\dagger}(x',t'))$ <br>  $G(x,t; x', t') = \frac{Tr(e^{-B(H-\mu V)} S(C) \hat{\psi}(x,t) \hat{\psi}^{\dagger}(x',t'))}{Tr(-e^{-B(H-\mu V)} S(C))}$  $(10.103)$  $Tr(e^{-\beta(H-\mu N)} S(C))$ The reason for the denominator will be made clear in the next section 10.3 Schwinger-Dyson Equations In this section, we consider a collection of particles that are mutually interacting via a two-body potential. We also assume that an external potential is present. This external potential defined in imaginary time in the interval  $[0, -i\beta\hbar]$  may be set to zero at the end to make the whole system translationally invariant in space and time so that we may then extract the self-energy function of the quasi particles, which Field Theory  $242$ is the real intention of this section. Alternatively, one could regard the external

So, basically this just tells you more details about non equilibrium Green's function and finally, there will be something called the Schwinger Dyson equation which is a very powerful basically a functional differential equation for the Green's function of a many body system. So, it is interesting to know that it is possible to write down those kinds of equations for the Green's function of many body system.

So, I will be just explaining all those things one by one and the problem is that you would not be able to solve any of these equations you will just be able to derive the equations and solving them is very very hard those are all topics of research. So, nobody knows how to solve them fully. So, you can still do some tentative type of approximation and check against some numerical simulation that is the best you can do.

So, this course is more about telling you what sort of questions are worth asking. So, this course does not provide any answers it just tells you what questions are worth asking. So, ok, I am going to stop here in the next class I will continue with Nonequilibrium Green's function.