Dynamics of Classical and Quantum Fields: An Introduction

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Green Functions in Grand Canonical Ensemble

Lecture - 41

Matsubara Green functions - II

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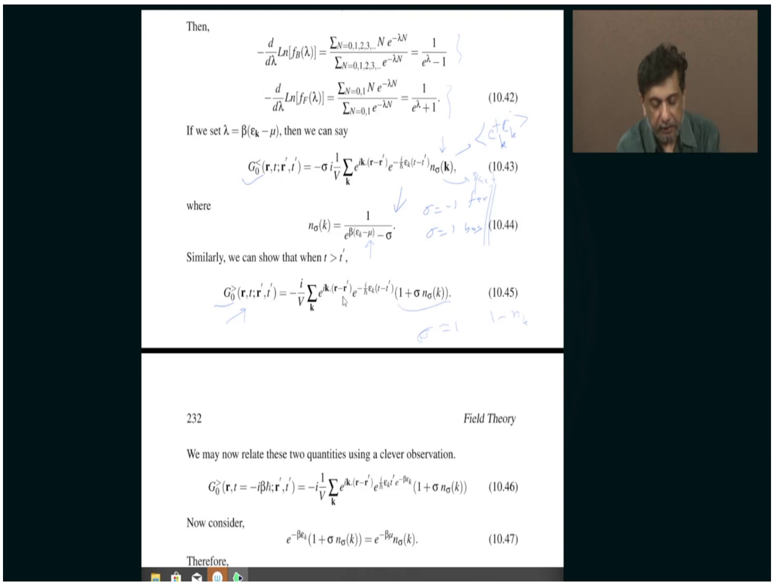

Ok, so, today let us see if we can make more sense out of these Matsubara Green's functions.

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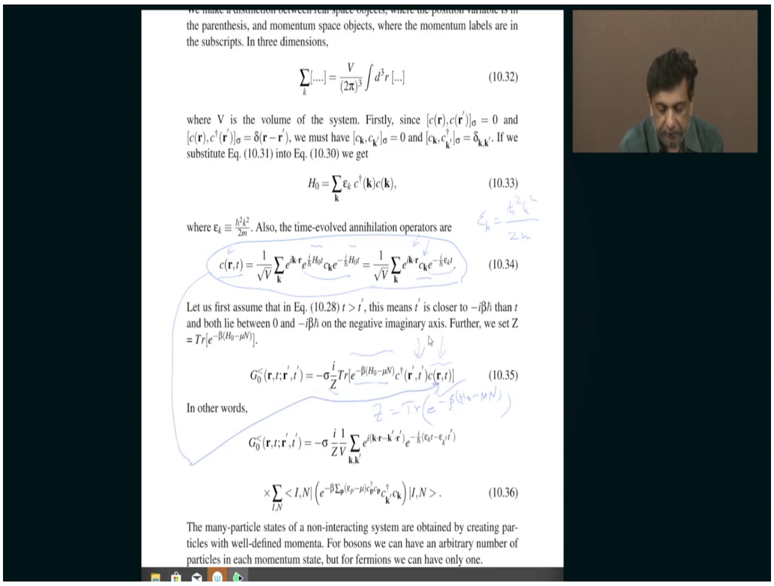

So, remember I told you that I still have to fulfil my promise of making sense of this original definition namely this that. So, I have not made sense out of claims such as this and I have to explain what; that means, physically, but in some sense well you can roughly convince yourself that this makes sense in the following way.

See, after all first of all it is obvious that this corresponds to a hole propagator; that means, you are first creating a hole because you are removing an electron at position or whatever that particle is provisionally I am going to assume the electrons because, that is typically the type of particles that we commonly encounters in solid state physics. That is electrons those are the ones that participate in electronic properties basically that is why it is called electronic properties because it is determined by how the electrons behave in the solid.

So, in any event so, the basically it is the electron that is being annihilated here at position r and t. So, in other words you are creating a hole first and then you are seeing how that hole racks have hooked in the system by running around here and there. And then eventually you remove the hole by or you fill the hole by inserting an electron at some other position r dash and at some other time t dash.

So, the point is that remember that in the old way of when I started off discussing the hole propagator I simply computed the overlap between the initial and final states.

But, now because the system is not isolated it is in contact with surroundings I have to take into account the fact that not all states mean the system is not going to be in a well-defined eigen state of the Hamiltonian to begin with anyway.

So, it is basically going to be in a superposition of all the eigenstates with some each state comes with a Boltzmann weight and if I also allow for the possibility of particles being exchanged with the surroundings then I also have this chemical potential. So, this is the grand canonical, so instead of the Boltzmann weight I have this grand canonical version of the Boltzmann weight.

So, I end up tracing the so, in other words rather than calculating the expectation value of c dagger c I end up first multiplying it by the Boltzmann weight or the grand canonical version of the Boltzmann weight which is e raise to minus beta H naught minus mu N and then I divide by the normalization which is basically the trace of e raise to minus beta H naught minus mu N.

So, that makes some sense, does not it? So, basically we have it makes sense because it certainly represents a whole propagator, but it also conforms to the fact that you are averaging over a whole bunch of states of the eigen states of the Hamiltonian each associated with an appropriate weight, which signifies how strongly the system is coupling to its environment ok.

So, if you are satisfied with that intuitive explanation in fact, one should not underestimate the value of intuitive explanations because lot of physics I mean a lot of formalism can be anticipated and in fact, a lot of unnecessary detailed calculations can be shortened or side stepped through use of physical intuition. So, one should not underestimate the role of physical intuition in simplifying calculations in physics.

In any event bottom line is that this is what it is, but now you see, what I am going to do is that I am going to try and convince you that if I decide to ignore the mutual interaction between particles then clearly the momentum becomes a good quantum number.

And I am perfectly justified in expanding the fields in plane waves so; that means, I am perfectly justified in doing this. So, I am perfectly justified in writing c of r comma t. So, in other words I am perfectly justified in writing the r dependence as a superposition of plane waves and this is the amplitude.

But more interestingly because it is a free particles because it is a free particle the time dependence of this operator is simply given by the time evolution with respect to the energy of a free particle. So, and what is the energy of the free particle? It is just h bar squared k squared by 2 m because p squared by 2 m and h p is h bar k and k is your wave vector.

So, it is as simple as that, you see so for a free particle things are incredibly simple that spatial dependence of course, will involve sum over plane waves, but then the time dependence will be determined by the space dependence because it is a plane wave and the dispersion relation is fixed because it is just p squared by 2 m. So, if given that I am currently only interested in free particles then I can very safely go ahead and insert this here and it is adjoint here and then see what I get.

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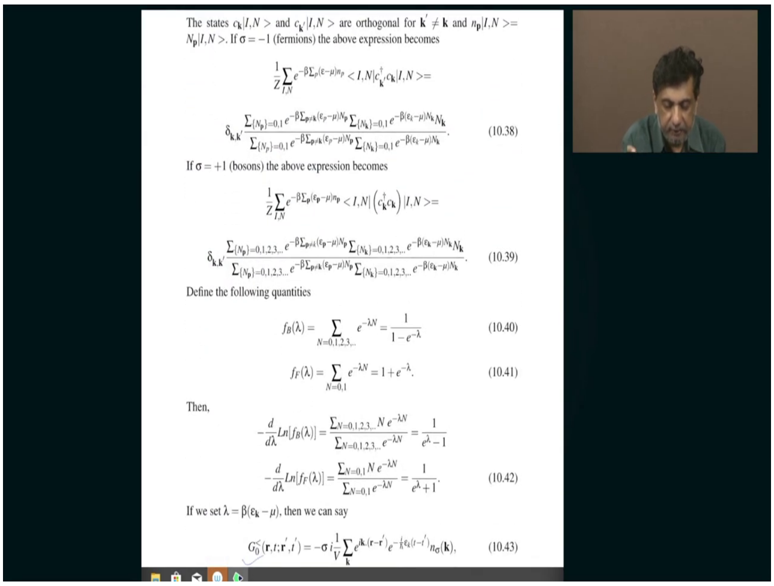

And what I get these intermediate steps are for you to be convince that this grand canonical ensemble in fact, leads to the same formulas if you know sum over all the number of particle and so on you end up with the Fermi - Dirac distribution and so forth.

But you see, even otherwise you are going to be convinced because what is going to happen is that you see if I take c dagger c I will just end up getting. So, and I am taking the trace here in fact, that is exactly what I have done here. So, when you take trace this this becomes a Kronecker delta. So, basically you will have to do this and take trace. So, you have to first insert that here and then you have to take trace over all the particles.

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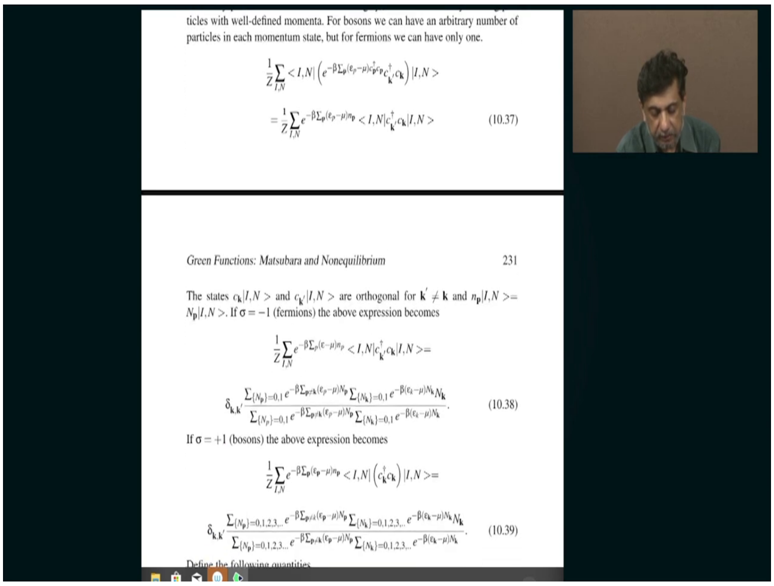

And for taking trace you have to choose a basis in which it is the number of particles is basically diagonal in the number of it is a particle number basis. So, I mean these are not unnecessary intermediate steps they are actually very crucial intermediate steps, but that they are somewhat annoying and tedious.

But the end result is quite expected and it kind of is very tempting to simply write this result, but you should keep in mind that it is strictly speaking it has to be derived this way by going all the way from here to here, but having obtained this result it is kind of believable it is so believable that it is tempting to ignore the derivation.

So, basically what this says is that the hole Green's function is simply related to your average of your particle number; that means, the average number of particles with momentum k. So, that is all it says that basically it is the Fourier transform of the average number of particles in momentum state k. So, that is the physical meaning of the hole Green's function in momentum space.

So, now you see it is general enough to accommodate both fermions and bosons if you select sigma is minus 1 you get fermions if you select sigma equals 1 you are describing bosons, but keep in mind that we are still working in the grand canonical and symbol. So, that is the chemical potential you have to keep dragging along all over the place, but as I told you repeatedly you see in stat mac if your system sizes are large. So, you can still study a canonical ensemble symbol which is more typical by just relating the chemical potential to the average number of particles.

So, you just calculate the average number of total particles and then you can relate the chemical potential to the average density of particles in your system. So, you might think that you know how does that correspond to canonical ensemble, because in the canonical ensemble the there is no such thing as average number of particles.

The number of particles is strictly fixed, but the claim is that you know when system sizes are large it is also fixed even in the grand canonical ensemble because even though in principle the number of particles in the grand canonical ensemble can fluctuate, but those the sizes of that fluctuations are extremely tiny compared to the average number of particles.

So, in fact, even in the grand canonical ensemble it is safe to say that the number of particles is fixed in the thermodynamic limit. So, that is the reason why the grand canonical ensemble becomes equivalent to the canonical ensemble in the thermodynamic limit. So, similarly you can ask yourself what would happen if you had a an electron Green's function; that means, you decided to first create an electron and then propagate it and then you destroy it.

So, clearly you get a different function which corresponds to the number density of holes. So, this is the number this is the particle number density, well in some sense it is yeah, this is the number of density of the actual electrons this is the number of density of whatever remains. So, if sigma is minus 1 is just 1 minus n k.

So, it is difference between this is the left over thing. So, the point is that if you add these two you are bound to get Dirac delta functions means you will rather you will get at t equal to t dash you are going to get a Dirac delta function ok.

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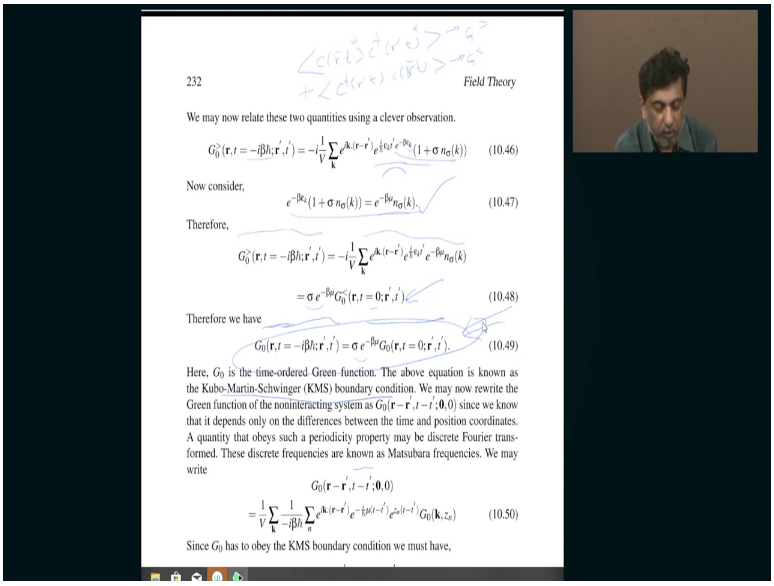
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We may now relate these two quantities using a clever observation.

$$G_0^>(\mathbf{r},t=-i\beta\hbar;\mathbf{r}',t') = -i\frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')} e^{\frac{i}{\hbar}\epsilon_k t'} e^{-\beta\epsilon_k}(1+\sigma\, n_\sigma(k)) \quad (10.46)$$

Now consider,

$$e^{-\beta\epsilon_k}(1+\sigma\, n_\sigma(k)) = e^{-\beta\mu} n_\sigma(k). \quad (10.47)$$

Therefore,

$$G_0^>(\mathbf{r},t=-i\beta\hbar;\mathbf{r}',t') = -i\frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')} e^{\frac{i}{\hbar}\epsilon_k t'} e^{-\beta\mu} n_\sigma(k)$$

$$= \sigma\, e^{-\beta\mu} G_0^<(\mathbf{r},t=0;\mathbf{r}',t'). \quad (10.48)$$

Therefore we have

$$G_0(\mathbf{r},t=-i\beta\hbar;\mathbf{r}',t') = \sigma\, e^{-\beta\mu} G_0(\mathbf{r},t=0;\mathbf{r}',t'). \quad (10.49)$$

Here, G_0 is the time-ordered Green function. The above equation is known as the Kubo-Martin-Schwinger (KMS) boundary condition. We may now rewrite the Green function of the noninteracting system as $G_0(\mathbf{r}-\mathbf{r}',t-t';\mathbf{0},0)$ since we know that it depends only on the differences between the time and position coordinates. A quantity that obeys such a periodicity property may be discrete Fourier transformed. These discrete frequencies are known as Matsubara frequencies. We may write

$$G_0(\mathbf{r}-\mathbf{r}',t-t';\mathbf{0},0)$$
$$= \frac{1}{V}\sum_{\mathbf{k}} \frac{1}{-i\beta\hbar}\sum_{n} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')} e^{-\frac{i}{\hbar}\mu(t-t')} e^{z_n(t-t')} G_0(\mathbf{k},z_n) \quad (10.50)$$

Since G_0 has to obey the KMS boundary condition we must have,

So, that is to be expected because that is going to correspond to either the average of the commutator or the anti commutator. So, basically if you have c dagger r dash t and then you decide to add c dagger r dash t c r t basically this will correspond to you know the particle Green's function and this is the hole Green's function. So, in some sense so, if you add these two it is just the anti commutator of c and c dagger which is clearly Dirac delta because it is the times are equal at equal times ok.

So, now, let us get to something little bit more interesting and that is I am going to point out that I am going to show you that there is a nice connection between G greater and G less and that connection is in fact, more general than what I have displayed here.

So, I have actually verified this for you know the Green's function of free fermions and free bosons, but notice that it is free bosons because you see the dispersion is h bar squared k squared by 2 m, but it does not have to. So, this so, called KMS boundary condition that I am now going to derive is more general it is applicable always ok.

So, the point is that if you take one of the times and decide to formally set it to minus i beta h bar. So, you might be wondering what right do I have to do that, but just you know just imagine that you forcibly set t to minus i beta h bar and just see what sort of algebraic expressions you get.

So, what you get is basically this expression becomes this expression. So, this one becomes this. Now, you exploit this identity because after all what is n sigma, n sigma is this because of this is the n sigma you can easily verify that this is valid. So, because of this you can go ahead and insert this instead of this ok.

So, when you do that low and behold this becomes the basically the hole Green's function because you started off with the particle Green's function and then you set one of the times to some very funny imaginary value of the time. And by selecting the proper imaginary value of the time you have succeeded in converting what is basically an electron Green's function into a hole Green's function but then that is back at time t equal to 0.

But, then there will be some pre factors there. So, that pre factors will have different signs depending whether you are dealing with fermions or bosons. So, if you are dealing with sigma equals minus 1 you are dealing with fermions and if it is plus 1 you are bosons. So, the bottom line is that this is called Kubo – Martin- Schwinger boundary condition.

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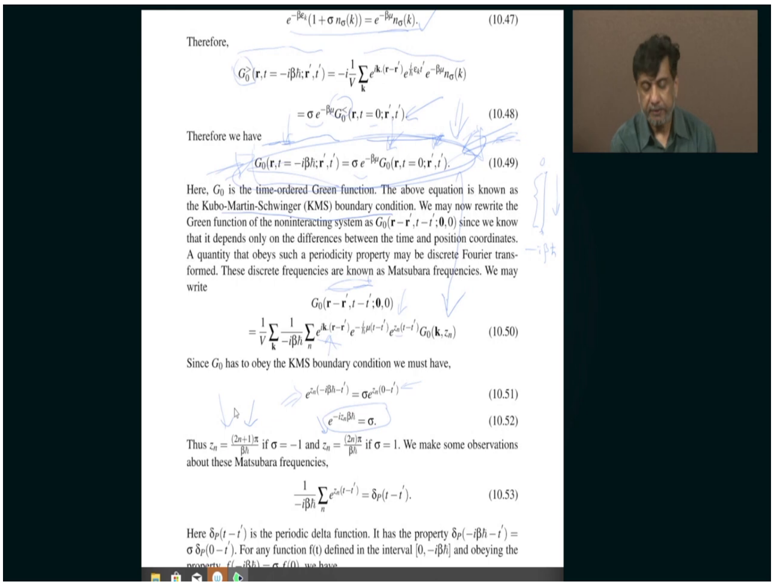

This is very important and in fact, we will be using this repeatedly in our discussions of Matsubara Green's function.

So, now that I have convinced you ok, I have not really convinced you that I have just derived you I have just derived this KMS boundary condition for the case of free particles, but I have not strictly convinced you that it is valid always. So, I told you that there are many things like this which I would not be able to explain you know I cannot explain everything in a lecture. So, some of these interesting questions I will have to either work it out in a special tutorial or I have to allow you to work it out in an actual exercise or an assignment ok.

So, that we will decide later on, but now let us provisionally accept that this is valid not only for free particles, but it is also valid in general. So, if it is valid in general then you see for a system that is in equilibrium clearly the most general form of the ok. Now, I have switched gears and I am speaking of time ordered Green's function I think somewhere down the road or even earlier I introduce the time ordering yeah.

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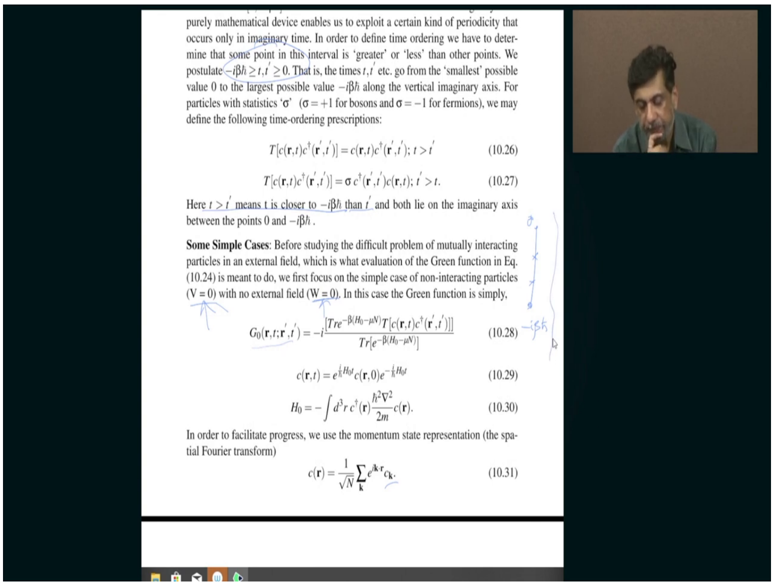

So, this time ordering remember I actually started off this way, I started off with time ordering and the time ordering is in this imaginary so, when the times are actually imaginary. So, I am going to continue that way. So, if the system is in equilibrium it is perfectly legitimate to think of the times as being on the imaginary axis.

And then once you decide once you commit to a certain type of Green's function whether it is particle or hole Green's function by selecting the order in which the t's and t dash occur, having done that after committing to a particle or a hole Green's function then of course, you can go ahead and analytically continue the times to a real times if you wish. But when you are dealing with this formal time ordering you are forced to imagine the times to be on the complex plane; that means, you are forced to imagine that the times are purely imaginary.

So, now you see given that. So, the reason why I have written it like this is because you see when t is minus i beta h bar it is clearly minus i beta h bar is the largest possible time because all the times lie in this interval and this is increasing this is the direction of increasing times. So, if t is minus i beta h G greater is basically same as G because after all what is G greater, G greater is basically the particle Green's function; that means, the annihilation to should be to the left of creation. So, you have to first create and then annihilate.

So, that means, that see the time ordering is automatically the same as particle Green function for this particular time. So, conversely if you are dealing with t equals 0 that is the smallest possible time. So, then the time order Green's function is automatically the hole Green's function, because see the time ordering now forces the greater time to come to the left and the greater time is the one that creates rather than annihilates.

So, then the creation comes to the left of the annihilation. So, you are first annihilating and then creating; that means, it is a hole Green's function. So, that is why this makes perfect sense ok. So, this this relation was relating the particle or electron particle Green's function to the hole Green's function, but this relates the time ordered Green's function to itself ok. So, that is the difference.

So, you see if this is the case then we know that basically in equilibrium the system is translationally invariant in both space and time. So, what; that means, is if you look at say if you look at the Green's function at point r and r dash; that means, you have either created or annihilated at r and you have annihilated or created at r dash, in that case if I shift my coordinate system to some other location. So, I just shift the origin of my coordinates without rotating or anything you just shift it parallel to itself to some other location.

So, then that r will go to r plus r 0 and r dash will also go to r dash plus r 0 because I have shifted by a fixed amount. So, then you see, clearly we do not expect the Green's function to depend on r 0 because the system is translationally invariant. So, it should only depend upon where r dash is relative to r; that means, if I sit at r it only matters where r dash is seen while sitting at r. So, it does not matter where the origin is that is pretty arbitrary.

So, therefore, the Green's function should clearly depend on the difference between r and r dash so, similarly with times as well. So, it should only matter what the duration that has elapsed between t and t dash. See, that those that is the duration between which you do the creation and the annihilation. So, it does not matter when you start or end basically the system is in equilibrium so, it should not matter.

So, if that is the case then clearly when I Fourier transform I will of course, as usual go with the plane waves because the system is translationally invariant, but then I can introduce certain frequency. So, you see normally when you do Fourier transform because the times are all continuous quantities. So, I should be doing a Fourier transform rather than a Fourier series because normally if you do not know the nature of the time dependence the most general thing to do is would be a Fourier transform.

But now we know that there is a sense in which the Green's function is has a flavour of being periodic because of this KMS boundary condition. So, the KMS boundary condition allows me to kind of relate these Green's function to something that is genuinely periodic.

So, if you have a Green's function that is in fact, genuinely periodic then we all know that such a Green's function can be written as a Fourier series instead of a Fourier transform. So, that is pretty much what this is. So, it is a series it is a series in discrete frequency. So, the frequency is now are no longer continuous they become discrete.

And now the question is now, what we have to do is we have to find out what those discrete frequencies are? So, in order to find that we of course, insert this relation into this supposed series expansion. So, when you do that you are forced to conclude that the as frequencies have to obey this sort of relation.

So, that means, this complex number of unit modulus should have this relation that is either plus or minus 1 so; that means, that basically the argument of this exponent should either be an odd multiple of pi if sigma is minus 1 or an even multiple of pi if sigma is plus 1.

So, in other words z n itself is an odd multiple of pi divided by beta h bar for fermions and it is an even multiple of pi divided by beta h bar for bosons.

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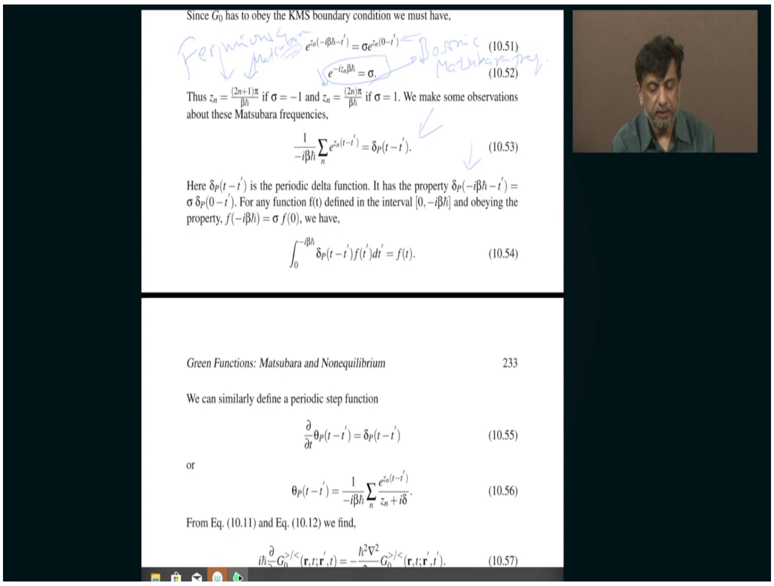

So, these are called bosonic and so, this is called the fermionic Matsubara frequency and this is called the bosonic Matsubara frequency. So, similarly your Dirac deltas also have to obey this bosonic fermionic periodic boundary conditions in imaginary time ok, because every function basically has to obey periodic boundary condition of the certain imaginary time because that is how it is ok.

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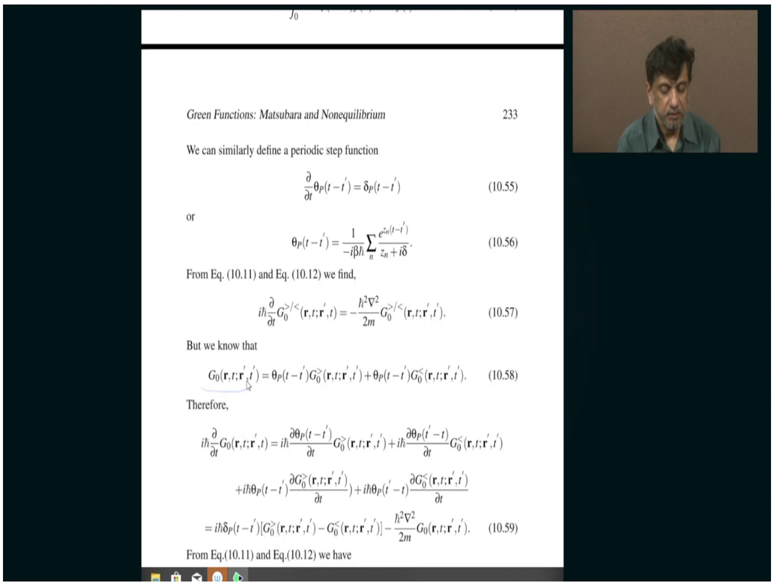

So, now, you can go ahead and convince yourself that the this G that I defined using this grand canonical statistical averaging of my you know particle and hole Green's functions; that means, by rather this particle hole operator c c dagger or c dagger c I average them out using grand canonical statistical averaging by inserting this weights. So, see, that kind of a physical definition will certainly give some quantity, but the big question is; does it deserve to be called a Green's function?

Or does it deserve to be called Green's function? Because the word Green's function is associated with the mathematician Green I forget the rest of the details, but I should probably look it up. But bottom line is Mister Green was a mathematician and he showed that his Green's function he had no inkling or understanding of many body theory, but he knew that his Green function always obeys this equation.

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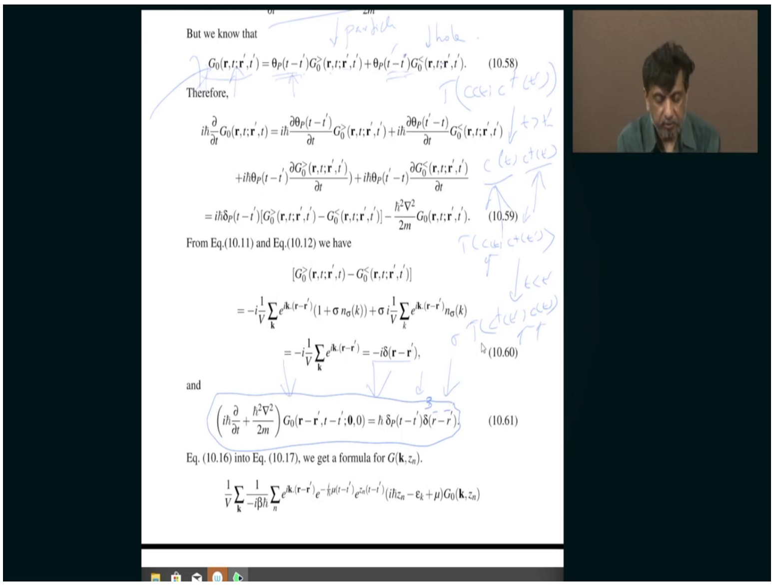

So, the question is that unless we can demonstrate that this quantum statistical definition of our so called Green's function which is obtained by quantum statistically averaging particle hole or hole particle creation operators, also obeys the same equation that Mister Green invented then only we have a right to call that Green's function.

So, what I have done in these lines is to demonstrate precisely that. So, I have been able to show that first of all this particle and hole Green's function trivially obey this, but then remember that because the time ordered Green's function are related to the particle and hole Green's function in this way, because you see if you are talking about the particle Green's function t is greater than t dash. Oh, sorry I made a mess it is t dash greater than t ok yeah one of them is t greater than t dash the other is t dash greater than t.

So; that means, if t is greater than t dash right. So, that means, your this is same as this; that means, if t is greater than t dash we are supposed to put whatever is greater on the left of whatever is smaller. So, so; that means, in effect what you are doing is you are first creating a particle and then annihilating it. So, G greater is basically the particle Green's function, conversely if you decide to make t less than t dash then you are supposed to put the thing which is smaller which is this one to the right. So, the greater should always to be to the left.

So, it will become like this and it will pick up a sign depending upon whether it is boson or fermion, because we know when you interchange you are supposed to pick up a sign if it is a fermion minus sign, if it is boson you pick up a plus sign which is same as not picking up a sign. So, bottom line is that if t is less than t dash you are supposed to first annihilate and then create.

So, it is a hole Green's function. So, basically this is particle and this is hole. So, your time ordering is basically some linear combination meaning it is either one or the other depending upon which one is greater ok.

So, but then see if you go ahead and formally try to see what equation what evolution equation this G 0 obeys then you immediately you will see that it obeys this equation because there will be a delta function in time, because you will be differentiating the step function which gives you delta function, but then the delta functions after differentiation that you get will force this to become t dash and it will force to add these two, but then adding these two with an appropriate sign, well actually they will subtract rather than add, but it will end up becoming this Dirac delta here ok.

So, bottom line is that this quantum statistical definition of the Green's function while not initially obvious that it deserves to be called Green's function with some effort you can show that in fact, it does deserve to be called a Green's function, because it obeys this equation ok.

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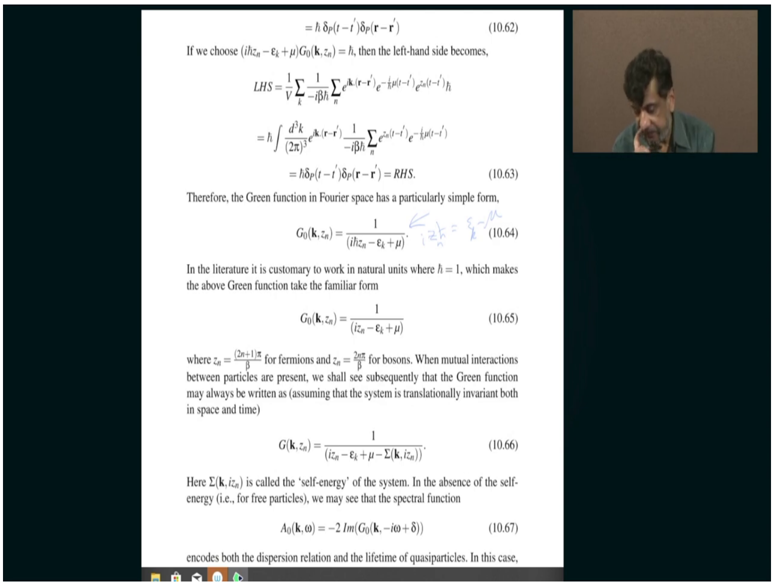

$$= \hbar\, \delta_P(t-t^{'})\delta_P(\mathbf{r}-\mathbf{r}^{'}) \qquad (10.62)$$

If we choose $(i\hbar z_n - \varepsilon_k + \mu)G_0(\mathbf{k}, z_n) = \hbar$, then the left-hand side becomes,

$$LHS = \frac{1}{V}\sum_k \frac{1}{-i\beta\hbar}\sum_n e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}^{'})} e^{-\frac{i}{\hbar}\mu(t-t^{'})} e^{z_n(t-t^{'})}\hbar$$

$$= \hbar \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}^{'})} \frac{1}{-i\beta\hbar}\sum_n e^{z_n(t-t^{'})} e^{-\frac{i}{\hbar}\mu(t-t^{'})}$$

$$= \hbar\delta_P(t-t^{'})\delta_P(\mathbf{r}-\mathbf{r}^{'}) = RHS. \qquad (10.63)$$

Therefore, the Green function in Fourier space has a particularly simple form,

$$G_0(\mathbf{k}, z_n) = \frac{1}{(i\hbar z_n - \varepsilon_k + \mu)}. \qquad (10.64)$$

In the literature it is customary to work in natural units where $\hbar = 1$, which makes the above Green function take the familiar form

$$G_0(\mathbf{k}, z_n) = \frac{1}{(iz_n - \varepsilon_k + \mu)} \qquad (10.65)$$

where $z_n = \frac{(2n+1)\pi}{\beta}$ for fermions and $z_n = \frac{2n\pi}{\beta}$ for bosons. When mutual interactions between particles are present, we shall see subsequently that the Green function may always be written as (assuming that the system is translationally invariant both in space and time)

$$G(\mathbf{k}, z_n) = \frac{1}{(iz_n - \varepsilon_k + \mu - \Sigma(\mathbf{k}, iz_n))}. \qquad (10.66)$$

Here $\Sigma(\mathbf{k}, iz_n)$ is called the 'self-energy' of the system. In the absence of the self-energy (i.e., for free particles), we may see that the spectral function

$$A_0(\mathbf{k}, \omega) = -2\, Im(G_0(\mathbf{k}, -i\omega + \delta)) \qquad (10.67)$$

encodes both the dispersion relation and the lifetime of quasiparticles. In this case,

So, then you can go ahead and convince yourself that this this coefficient you see this this is the Fourier coefficient of this G 0 the time ordered Green's function therefore, has this very simple interpretation ok.

So, it basically gives you is the reciprocal of a function or basically it is a it is an algebraic function which has poles so; that means, basically it. So, this function has poles whenever i h bar becomes E k minus mu. So, you see there are these simple poles. So, in that sense this Green's function is extremely simple and algebraic in its nature, but you see this is only for free particles because after all I have assumed that E k epsilon k is h bar squared k squared by 2 m.

So, you see k is anyway always good idea to introduce even when the system is not consisting of free particles. So, long as the system is translationally invariant k is anyway good quantum number, but then you see even though k is a good quantum number even when there are interactions in the system so, long as the system is translationally invariant epsilon k is not a good idea because epsilon k by definition is h bar squared k squared by 2 m, but that is only kinetic energy.

But then when particles interact with each other you also have potential energy so, you cannot really do this. So, the way to introduce that and then you see that the potential is anyway very dynamical because it is mutual interaction between particles.

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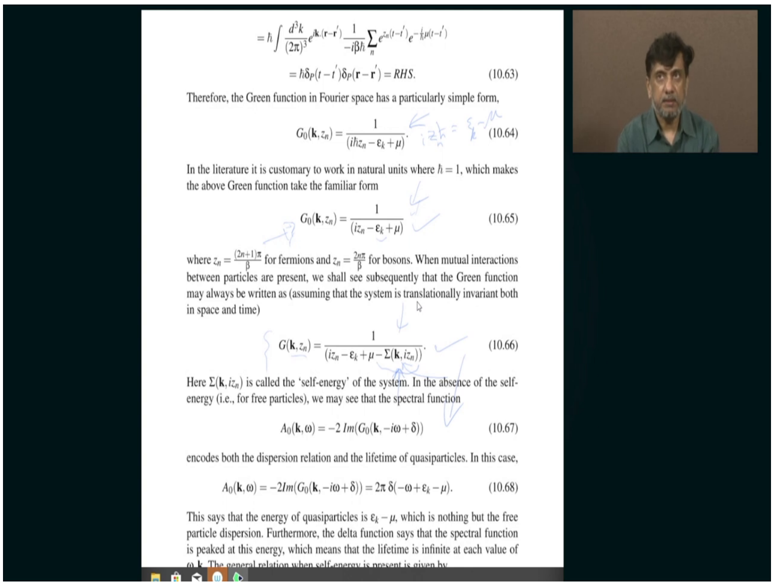

So, the way you introduce that is through what is called as self-energy rather than as writing epsilon k you postulate that there ought to be something else and after all what is that something else it cannot I mean it cannot be anything, but a function of k and z there is nothing else there. So, the most general situation is when you are able to write down some function of k and z n. So, it is customary to write it as this ok.

So, later on we will discuss some implications of these ideas you know what this means and how to go about calculating sigma, you see that is one of the central questions in many body theory how to calculate the self-energy of a system of interacting particles. So, it is by no means an easy task it is very difficult and there are many methods that people use there is something called the loop expansion. So, you have this single loop double loop and so on.

So, we will try to touch upon those issues we will not be doing full justice to those ideas because as I said this course is mostly about informing you about the topics that are worth learning it is not to fully teach you those topics, just tells you that these are the things that you should go ahead and learn ok.

So, I am going to stop here in the next class I will start from here, I will tell you what are the consequences of choosing either this or this you know there are some physical you know ramifications and implications of choosing this as your Green's function. We have not really chosen it we have derived it, but then this itself has some it is own intrinsic physical meaning which we can extract through it is real and imaginary parts ok.

So, and especially this the imaginary part of this quantity has an immensely important physical meaning, which I am going to discuss in the next class. So, I am going to stop here let us meet in the next class.

Thank you.