Advanced Condensed Matter Physics
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Lecture – 16
Finite temperature Green's function and Matsubara frequencies

We shall now talk about Finite temperatures because the experiments for condensed matter systems are always done at finite temperature. And an important goal of the physics that we are doing is to explain experiments or experimental data and for that we need to go to finite temperatures. So, far we have been talking about 0 temperature greens function.

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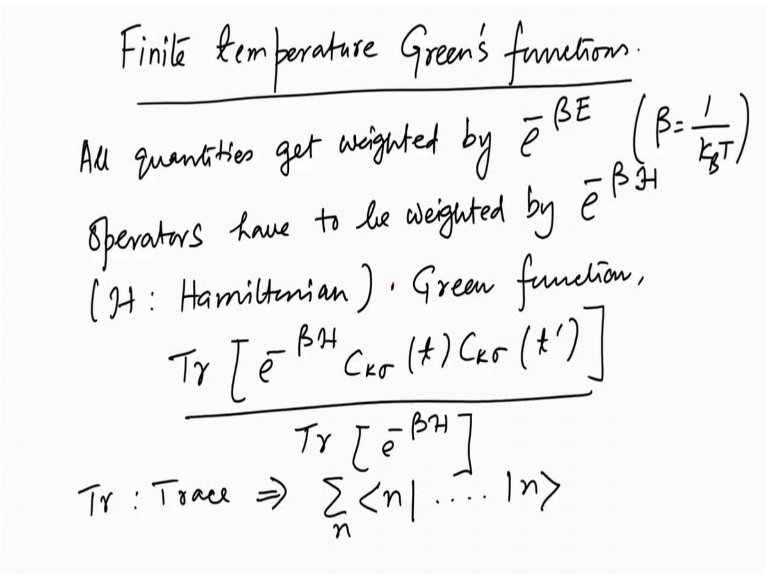

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And now we shall talk about Finite temperature greens functions.

So, what happens at finite temperature is that all quantities get wetted by the factor. So, by exponential minus beta e where beta equal to 1 over k t, which is called as the inverse temperature and k is the k with a subscript b is called as a Boltzmann constant. So, now, what happens to the operators at finite temperatures? So, which means that the operators have to be weighted by this operator where H is the Hamiltonian of the system.

So, now so, at finite temperatures the operators that we need to write down the greens function they have to be weighted by this quantity or the weighting factor which is exponential minus beta H beta being the inverse temperature or 1 over k t H is the Hamiltonian for the system.

So, we write down a greens function as. So, greens function will write down later, but it is written down as the trace of exponential beta H C k sigma t and C k sigma t prime divided by trace of exponential minus beta H.

So, this is the a form of the greens function and the trace implies the T r is actually the trace, which implies that we have to take the trace over the complete set of states n.

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$$C_{k\sigma}(t) = e^{i\mathcal{H}t} C_{k\sigma}(0)\, e^{-i\mathcal{H}t} \qquad H = H_0 + H'$$

$e^{\pm i\mathcal{H}t}$, $e^{-\beta H}$ → H' appears at both places

Matsubara (1955) $\quad \beta = \frac{1}{k_B T} \Rightarrow$ Complex time

$\boxed{\text{Time is treated as complex temperature}}$

occupation numbers

Bosons $\quad n_B = \left(\frac{1}{e^{\beta\hbar\omega_q} - 1}\right)$

Fermions $\quad n_F = \left(\frac{1}{e^{\beta\epsilon_k} + 1}\right)$

And the operators this is pretty much we are still at 0 temperatures. So, the operators are written as exponential i H t C k sigma 0 and exponential minus i H t H being the H 0 plus H prime right.

So, this we have seen and so, H prime now appears at two places. So, remember that we have done perturbation theory with in powers of H prime, now H prime is occurring at these plus minus i H t we have dropped a H cross the Planck's constant and it also appears at exponential minus beta H. So, this appears at both places we were writing a curly H does not matter. So, so H prime appears at both these places.

So, the perturbative expansion in terms of H prime was earlier included in this term. And should we now again do a perturbation expansion in terms of H prime with this. So, that is the question? Now the answer to this question was given by Matsubara in the year

1955 in which he realized that beta equal to one over k T can be considered as complex time.

So, if you consider this as complex time this beta then these two factors which are written here and here they can be combined together. And so, basically if they can be combined together, then we can do a single perturbation theory with respect to H prime and can write down the complete brains function or the full greens function in terms of that.

But what finally, was done is exactly the opposite time is regarded or treated as complex temperature; this is an important concept in the finite temperature calculations that will see henceforth. Another motivation of the Matsubara formalism so, we henceforth we call this as a Matsubara formalism is that the occupation numbers for bosons the occupation numbers which are the distribution.

So, these are bosons and fermions and this you know that this is written as exponential one divided by exponential beta H cross omega q minus 1, where omega q are the boson energies and this is written as exponential beta epsilon k plus 1 and where epsilon ks are the energies. So, these are the occupation numbers.

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Occupation numbers can be expanded in a series.

$$n_F(\xi_k) = \frac{1}{e^{\beta\xi_k}+1} = \frac{1}{2} + \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \frac{1}{\frac{(2n+1)i\pi}{\beta} - \xi_k}$$

$$n_B(\omega_q) = \frac{1}{e^{\beta\hbar\omega_q}-1} = -\frac{1}{2} + \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \frac{1}{\frac{2\pi n i}{\beta} - \hbar\omega_q}$$

Theorem $\Rightarrow$ Any meromorphic function may be expanded as a summation over its poles and residues at the poles.

$n_B \Rightarrow$ has poles at even multiples of π/β

$n_F \Rightarrow$ has poles at odd multiple of π/β $\Rightarrow$ which lie on the imaginary axis.

Churchill (Complex analysis)

Now these occupation numbers can be expanded in a series and let us call this 1 as n F let us call 1 this as n F and let us call this one as n B.

So, n F is written as which is as we have written earlier it is plus 1 this is written as a series half plus 1 over beta, sum over n equal to minus infinity to plus infinity and this is 1 divided by 2 n plus 1 i i pi by beta minus xi k and the n B for the energies omega q, which as we have written it down minus 1 this is equal to a minus half plus a 1 by beta n equal to minus infinity plus infinity divided by 2 pi n i by beta minus omega q or we can keep this H cross here or we can drop it later.

Now, these are the expressions for the occupation densities of the occupation numbers for the fermions or bosons, we will not provide proof for that a rigorous proof for that, but definitely we will tell you that it looks like that there are poles or singularities, if you are familiar with the complex analysis or the complex integration these are called as the poles.

So, there are poles at odd multiples of i pi by beta and these have poles at even multiply even multiples of pi over beta a this we will prove and we simply say that this comes from a theorem and the theorem states that, that any Meromorphic functions; please see the definition of meromorphic functions maybe expanded as a as a summation over it is poles and residues at the poles.

Let me box this thing I am simply taking the statement and using it to know more about this you can look at a complex analysis book by Churchill. So, what it says is that the boson occupation functions?

So, n B has a poles at poles at even multiples of pi over beta in the along the imaginary axis. So, let us n f it has poles at odd multiples of pi over beta, but which lie on the imaginary axis ok.

So, these are even things are 2 2 n pi i by beta and this is 2 n plus 1 pi i by beta.

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Both the summations can be written as:

$$\sum_n \frac{1}{i\omega_n - \omega_q} \quad \text{and} \quad \sum_n \frac{1}{i\omega_n - \xi_K}$$

(Boson) (fermion)

Non interacting Green's function $\Rightarrow \dfrac{1}{i\omega_n - \xi_K}$

$\rightarrow$ Matsubara Green's function.

Time is a Complex quantity $\tau = it$
(imaginary)

Green's functions are functions of τ bounded between $[-\beta : \beta]$

So, both the summations it is apparent that can be written as 1 sum over n 1 divided by i omega n minus omega q this is for bosons and this is again a sum over n i omega n minus xi k, this is for or xi q does not matter I mean the momentum index does not matter for fermions. So, this is for bosons and these are for fermions.

So, for fermions they are odd integers of pi over beta and for bosons there even integers of pi over beta. Now it is interesting to note that at this form either of the forms they correspond to a non-interacting greens function, function is of the form 1 divided by i omega n minus xi k and this non interacting greens function is called as the Matsubara greens function. Matsubara is a Japanese physicist.

So, now, in the Matsubara formalism as we have said the time is a complex quantity and it is actually written as it is actually an imaginary quantity if you, it is a and which is written as tau equal to i t and the greens functions these greens functions the Matsubara greens functions are functions off of tau and bounded between minus beta 2 beta 2 plus beta.

So, that is the range of tau for the Matsubara greens functions which are so, tau is nothing, but the time, but it is just that it is a complex time and these greens functions are functions of these tau bounded between minus beta 2 plus beta. Now let us take any function which is a function of tau and 1 bounded between these values minus beta and plus beta we can always do a Fourier series.

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Take an arbitrary function $f(\tau) \Rightarrow$ expanded in Fourier Series.

$$f(\tau) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi\tau}{\beta}\right) + b_n \sin\left(\frac{n\pi\tau}{\beta}\right)\right]$$

Where the coefficients a_n and b_n are defined by,

$$a_n = \frac{1}{\beta}\int_{-\beta}^{\beta} d\tau\, f(\tau) \cos\frac{n\pi\tau}{\beta}$$

$$b_n = \frac{1}{\beta}\int_{-\beta}^{\beta} d\tau\, f(\tau) \sin\frac{n\pi\tau}{\beta}.$$

Look at Arfken, Kreyszig

$$f(i\omega_n) = \frac{1}{2}\beta(a_n + i b_n)$$

So, take an arbitrary function f tau, which can be expanded in Fourier series of the form. So, f of tau equal to half of a 0 plus n equal to 1 to infinity we have a a n cosine n pi tau over beta and plus b n sine n pi tau over beta.

So, where the coefficients a n and b n are defined by a n equal to 1 over beta minus beta 2 plus beta as we said that is bounded by minus beta n plus beta. So, this is f of tau and a cosine of n pi tau over beta whereas, the be n is exactly the same thing, but with the sine term f of tau and the sine n pi tau over beta. Look at Arfken mathematical physics book or kreyszig for information on these Fourier series.

So, in a compact notation we can write f of i omega n this is equal to half of beta a n plus i b n. So, this is the rather the so, this is f as a function of these frequencies that we had talked about and which can be obtained from the Fourier transform of f tau in the following fashion.

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$$f(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-in\pi\tau/\beta} f(i\omega_n)$$

$$f(i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\, f(\tau)\, e^{i\pi n\tau/\beta}.$$

<u>Boson</u> $f(\tau) = f(\tau+\beta)$ for $-\beta < \tau < 0$

<u>Fermion</u> $f(\tau) = -f(\tau+\beta)$ for $-\beta < \tau < 0$

So, f tau is related to the f i omega n as n equal to minus infinity to plus infinity exponential minus i n pi tau by beta f of i omega n, such that our f of i omega n is nothing, but it is equal to half of minus beta 2 plus beta d tau f of tau exponential i pi n tau over beta.

So, these are the properties of these functions, we shall later show that these functions are nothing, but the greens function the Matsubara greens function that we are going to talk about and as said earlier that these functions are needed in order to have the experimental quantities, which are always done at finite temperatures.

So, there are further simplifications possible and for bosons the simplifications are like this that we have an additional property, which is equal to f tau equal to f tau by tau plus beta for minus beta to be in the range for tau to be in the range minus beta and 0.

And so, this is a sort of periodicity of the function tau we are going to show that and for fermions, we are we have an anti-symmetric situation in which we so, this is in again in the limit tau to be between minus beta and 0 and let us show this for bosons.

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Bosons

$$f(i\omega_n) = \frac{1}{2}\left[\int_0^\beta d\tau\, f(\tau)\, e^{i\pi n\tau/\beta} + \underbrace{\int_{-\beta}^{0} d\tau\, f(\tau)\, e^{i\pi n\tau/\beta}}_{\tau \to \tau+\beta.}\right]$$

$$f(i\omega_n) = \underbrace{\frac{1}{2}\left(1+e^{in\pi}\right)}\int_0^\beta d\tau\, f(\tau)\, e^{in\pi\tau/\beta}.$$

$$f(i\omega_n) = 0 \text{ for } n \text{ to be odd.}$$

$$f(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} f(\tau) \qquad \omega_n = \frac{2n\pi}{\beta}.$$

$$f(\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} f(i\omega_n)$$

So, f of i omega n equal to half of 0 to beta d tau I am splitting the minus beta 2 plus beta integral from 0 to beta and minus beta to 0. So, this is the first term f tau and exponential i pi n tau over beta and plus a minus beta to 0 d tau f tau exponential i pi n tau over beta. And now if we change the variables in this term in this term if we change variable from tau to tau plus beta, then I get f of i omega n to be half of 1 plus exponential i n pi from 0 to beta d tau.

So, both of them can be combined to write it in this thing 1 should check this n pi tau over beta. So, because of this first factor here f of i omega n equal to 0 for n to be n to be odd thus for bosons we can write it as f of i omega n equal to 0 to beta d tau, exponential i omega n tau f of tau and for omega n to be even number because for odd it is equal to 0.

So, 2 n pi by beta. And similarly your f tau becomes equal to 1 over beta sum over n, but now n is denotes only odd sorry only even integers and this is minus i omega n tau, n integer means the omega n will correspond to even factors or rather even multiples of pi over beta that is what. So, n is restricted in that sense.

F of i omega n so, this is for fermions; So, we have used this property which is because the tau going to tau plus beta, then we have used that f tau of beta equal to f tau and have written down this second term; here and this second term becomes equal to 0 if n is equal to odd and that is why the Bosonic frequencies are even multiples of pi over beta. Let us see these for fermions.

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Fermions

$$f(i\omega_n) = \frac{1}{2}\left(1 - e^{in\pi}\right)\int_0^\beta d\tau\, f(\tau)\, e^{in\pi\tau/\beta}.$$

$f(i\omega_n) = 0$ if n is even.

$$\left.\begin{aligned} f(i\omega_n) &= \int_0^\beta d\tau\, e^{i\omega_n\tau} f(\tau) \\ f(\tau) &= \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} f(i\omega_n) \end{aligned}\right\} \quad \omega_n = \frac{(2n+1)\pi}{\beta}.$$

Limit to zero temperatures can be taken by analytic continuation of $i\omega_n \to \omega_n + i\eta$

For fermions we have this odd property and then I will again split up the sum or rather the integral into 2 terms, which is half 1 minus exponential i n pi. Again I will do the same trick of writing down the minus beta over 0 to will change the variable from tau 2 tau plus beta and use the anti-symmetric property of f of tau with respect to f tau plus beta and this is equal to; So, d tau f of tau exponential i n pi tau over beta all right.

So, now it says that f of i omega n equal to 0 if n is even for n to be odd we have f i omega n. So, we have omega n to have only odd values of pi over beta.

So, this is going to be 0 to beta d tau exponential i omega n tau f of tau and f of tau, the Fourier transform of that is equal to 1 over beta sum over n exponential minus i omega n tau f over i omega n and for these things omega n equal to 2 n plus 1 pi over beta ok.

So, these are things that we have learned now we have written down that f is an arbitrary function, but; however, that arbitrary function having some symmetry it tells us that there are these the frequencies for fermions and bosons they get quantized or rather they are discrete in terms of either even multiple for pi over beta for bosons and all multiple odd multiples of pi over beta for fermions.

So, these Fourier these functions will be shown these arbitrary functions f will be shown as the greens function. And the merit of the Matsubara greens function is that it directly leads to physical results such as the electrical properties such as conductance or transport properties such as conductance or you know magnetic properties such as magnetic susceptibilities etcetera and they are complex functions of i omega n as you can see here. And now if you need to go to 0 temperatures, then 1 can do an analogy continuation. So, will write this limit to 0 temperatures can be taken by analytic continuation of i omega n to omega n plus i eta this is eta.

So, eta goes to 0. So, you need to a plus or minus depend on whether we want to go to. So, this is for the retarded greens function and which are directly related to the experimental data. So, we have extended the 0 temperature formalism for an arbitrary function to finite temperature and found that, the there are restrictions or conditions on the frequencies for bosons and fermions and these show up in the form of poles of the Matsubara greens function and we shall now define the greens function themselves.

So, let us write down the Matsubara greens functions.

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Matsubara Greens functions.

Fermions

$$\mathcal{G}(k,\tau,\tau') = -\langle T_\tau\, c_{k\sigma}(\tau)\, c^{+}_{k\sigma}(\tau')\rangle$$

T_τ : Time ordering operator which arranges Fermionic operators such that earliest τ (closest to $-\beta$) is put at the extreme right.

$$\mathcal{G}(k,\tau,\tau') = -\Theta(\tau-\tau')\,Tr\left[e^{-\beta(K-\Omega)}e^{\tau K}c_{k\sigma}e^{-(\tau-\tau')K}\right] + \Theta(\tau'-\tau)\,Tr\left[e^{-\beta(K-\Omega)}e^{\tau' K}c^{+}_{k\sigma}e^{(\tau-\tau')K}c_{k\sigma}e^{-\tau K}\right]$$

$\underbrace{K = H-\mu N}_{\text{operator}}$ $\quad \Omega$: Grand $\underbrace{\text{potential}}$ $\rightarrow$ scalar $= -k_B T \ln Z_G$

So, let us write start with the electron Matsubara greens function, but as we know that the only difference comes in the way the frequencies are quantized. So, we would only write down for the electron or the fermions, let us write down for the use the word fermion rather than electron.

So, the fermions we write it down for, but essentially you can write it down almost similarly very similarly for the bosons as well. Here we will use a curly G a calligraphic

G to denote the greens function and to distinguish it between with this with the 0 temperature greens function.

So, we have a 2 time involved and which is written as a minus t tau and a C k sigma tau and a C k sigma dagger tau prime. So, now, the 2 times are involved or rather complex times are involved and we have taken 1 k 1 can taken a k and a k prime and write the 2 operators fermion operators with k and k prime that would not change anything.

Important thing is that we shall show that the greens function identically depends on tau minus tau prime and not tau and tau prime individually, thus at the end 1 can drop 1 of the time indices and can write the resultant greens function as a function of 1 time only will have to come to that.

So, let us write down k tau and tau prime. So, as we said that this will be written down in terms of the trace and this t tau is again the time ordering operator, which orders the time that is earliest time tau earliest tau to be closest to minus beta.

Now, this is the difference between the 0 temperature greens function that we do not have a minus infinity here, if the tau is bounded between minus beta to plus beta which is why all these properties symmetry properties of the bosons and the fermions came.

So, will write this once more that let us before we write down the greens function let us at least define the T tau a time ordering operator which arranges, which arranges the fermionic operators such that the earliest tau, tau closest to beta closest to minus beta is put at the extreme right.

So, this is a definition of the time ordering operator and so, it serves the same purpose as the time ordering operator in 0 temperature formalism excepting that that was pushed to minus infinity or plus infinity, here it is pushed towards the 1 extremity which is beta I mean minus beta in this particular case.

So, we keep using the calligraphic greens g for denoting Matsubara greens functions. So, we have the left hand side is written with 2 time indices the tau indices will see that how these 2 time indices can eventually be dropped? For that let us write down k as tau tau prime the so, the time ordering can be trivially taken into account by the theta operators, which we have learnt that tau is greater than tau prime this is equal to 1 this function is equal to 1 else it is equal to 0. And trace of exponential minus beta k minus omega exponential tau k C k a sigma exponential minus tau minus tau prime k i will tell you what k is.

And there is another term which is equal to so, this and there is another term which is equal to tau prime minus tau trace of exponential minus beta k minus omega all these ks omegas will be said just in a while k and then C k sigma dagger exponential tau minus tau prime k C k sigma exponential minus tau k you should write this neatly and see for yourself.

Now this k is an operator. So, k equal to H minus mu n where H is the Hamiltonian of the system and we decide to work in the grand canonical ensemble that is why this chemical potential has been used mu is the chemical potential and is the number of particles.

And this omega is called as the grand potential and this grand potential is the basically the just like the free energy in canonical ensembles. So, the k t log z would give us a free energy and this is actually the k t minus k t log Z G, where Z G equal to just write it where Z G is the partition function in the grand canonical. So, this G corresponds to this G corresponds to the grand canonical ensemble.

So, remember that this is an operator while this is a scalar quantity and this distinction will be needed in the subsequent discussion. So, now, we shall use a theorem of the cyclic variation. So, it says that the trace is unchanged by a cyclic variation of the operators.

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Trace is unchanged by a cyclic variation of the operators, i.e.

$$Tr(ABC) = Tr(BCA) = Tr(CAB)$$

$e^{-\beta\tau}$ or $e^{-\beta\tau'} \rightarrow$ to the left.

$$G(k, \tau-\tau') = -\Theta(\tau-\tau')\, Tr\left[e^{-\tau' k} e^{-\beta(k-\Omega)} e^{\tau k} c_{k\sigma} e^{-(\tau-\tau')k} c^{\dagger}_{k\sigma} \right] + \Theta(\tau'-\tau)\, Tr\left[e^{-\tau k} e^{-\beta(k-\Omega)} e^{\tau' k} c^{\dagger}_{k\sigma} e^{-(\tau'-\tau)k} c_{k\sigma} \right]$$

Commutation $\quad e^{-\tau' k} e^{-\beta(k-\Omega)} = e^{-\beta(k-\Omega)} e^{-\tau' k}$

That is so, trace of A B C is equal to trace of B C A is equal to trace of C A B and so on.

So, these are cyclic cyclically changing the traces the trace remains invariant. So, what we why we said is that we want to use the exponential minus beta tau term or exponential minus beta tau term tau prime term push it to the left. So, that G k there is another thing that has been achieved is that the right hand side is completely a function of tau minus tau prime.

So, we can start writing down the left hand side to be a function of tau minus tau prime and this is equal to a minus theta tau minus tau prime, it is just mathematically a little cumbersome, but there is nothing very difficult about it you can have to just do it 1 once by yourself to get convinced.

And there is a trace that is there exponential minus k exponential minus beta k minus omega exponential k this tau k and then there is a C k sigma I should have written it in 1 line exponential minus tau minus tau prime k and the C k sigma dagger and then there is this plus theta tau prime minus tau and trace and exponential minus tau, k exponential beta k minus omega an exponential tau prime k and C k sigma dagger exponential minus tau prime minus tau k C k sigma.

So, these are the 2 terms where we have used the cyclic variation of the trace. Now consider the commutation of these 2 operators. Now there is the operator in these 2 terms the 2 exponential a k only because as I said omega is a scalar quantity. So, these 2 operators are both k in the 1 is with the exponential minus tau t the other is with minus beta k. So, they should commute. So, commutation says that exponential minus tau prime k exponential beta k minus omega and same with tau or tau prime does not matter in either of the terms the first term there is a tau prime

So, we have written down here an exponential minus beta k minus omega an exponential minus tau prime k. So, these are the commutation and now we can use this commutation relation and can push the exponential k minus omega to the other side.

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$$\mathcal{G}(\vec{k}, \tau-\tau') = -\Theta(\tau-\tau')\,\mathrm{Tr}\left[e^{-\beta(K-\Omega)}\, e^{(\tau-\tau')K} c_{k\sigma}\, e^{-(\tau-\tau')K} c^{\dagger}_{k\sigma}\right]$$
$$+\,\Theta(\tau'-\tau)\,\mathrm{Tr}\left[e^{-\beta(K-\Omega)}\, e^{-(\tau-\tau')K} c^{\dagger}_{k\sigma}\, e^{(\tau-\tau')K} c_{k\sigma}\right]$$

Since $\mathcal{G}$ depends on $\tau-\tau' \to$ drop one variable:

$$\mathcal{G}(k,\tau) = -\langle T_\tau\, c_{k\sigma}(\tau)\, c^{\dagger}_{k\sigma}(0)\rangle$$
$$\mathcal{G}(k,\tau) = -\mathrm{Tr}\left[e^{-\beta(K-\Omega)}\, T_\tau\left(e^{\tau K} c_{k\sigma}(\tau)\, e^{-\tau K} c^{\dagger}_{k\sigma}(0)\right)\right]$$

Now consider $\underline{\tau < 0}$ use $f(\tau) = -f(\tau+\beta)$
$(-\beta < \tau < 0)$

And write down the G as k tau minus tau prime minus theta of tau minus tau prime and the trace of exponential minus beta k minus omega exponential tau minus tau prime k C k C k sigma exponential minus tau minus tau prime k C k sigma dagger and there is another term, which is theta tau prime minus tau trace of exponential minus beta k minus omega exponential minus tau minus tau prime k k C k sigma dagger exponential tau minus tau prime k C k sigma.

So, that is the greens function and since as we have been saying that they depends upon tau minus tau prime on both the sides drop 1 index 1 variable rather.

So, now that tells us that k tau it is equal to minus T tau C k sigma tau and C k sigma dagger 0, because we are talking about just 1 time which is equal to minus trace of exponential minus beta k minus omega, T tau of exponential tau k C k sigma tau tau C k sigma tau exponential minus tau k C k sigma tau a 0 I am sorry 0 and so on.

So, this is the form of the greens function finally, which is what we have been trying to get at it is a Matsubara greens function a function of I mean we have taken this to be k it could be any suitable quantum label for the problem. And now consider these additional symmetry properties that we have so, considered tau to be between minus beta and 0; that means, consider tau to be negative and use the property f tau to be minus f tau plus beta.

We have been telling this that those arbitrary functions can actually be like our greens functions, which are relevant for us and in this limit of minus beta less than tau less than 0.

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$$\mathcal{G}(k,\tau) = \mathrm{Tr}\left[e^{-\beta(K-\Omega)} c^{\dagger}_{k\sigma} e^{\tau K} c_{k\sigma} e^{-\tau K}\right]$$

Use cycling invariance of Trace

$$\mathcal{G}(k,\tau) = \mathrm{Tr}\left[e^{\beta\Omega} e^{\tau K} c_{k\sigma} e^{-(\tau+\beta)K} c^{\dagger}_{k\sigma}\right]$$

$e^{\beta\Omega}$ is not recycled

$$\boxed{K = H - \mu N}$$

Adjusting $e^{\pm\beta K}$.

$$\mathcal{G}(k,\tau) = \mathrm{Tr}\Big[e^{-\beta(K-\Omega)} \underbrace{e^{(\tau+\beta)K} c_{k\sigma} e^{-(\tau+\beta)K} c^{\dagger}_{k\sigma}}_{-\mathcal{G}(k,\tau+\beta) \text{ for } -\beta<\tau<0}\Big]$$

Then we can write down the G k tau to be equal to trace of exponential minus beta k minus omega and C k sigma dagger exponential k C k sigma exponential minus tau k and that is the form of the greens function. And now 1 can use that cyclic property of trace several times and can write it down as.

So, will write this give this clue here use cyclic invariance of trace G k tau equal 2 equal to trace of trace of exponential beta omega exponential tau k, tau k C k sigma, exponential minus tau plus beta k and C C k sigma dagger and so on.

And so, exponential beta omega is not recycled, because it is not an operator. Recycle means it is not just the way the trace of a b C and b C a that it has not been done it has been kept, where it is it has not been recycled and then finally, I mean one can do a regrouping by adding a adjusting exponential plus minus beta k, we have written down as G k tau equal to trace of exponential minus beta k minus omega exponential tau plus beta k remember K equal to H minus mu n.

So, this is our Hamiltonian now and this and then C k sigma exponential minus tau plus beta k C k sigma dagger. And so, this is the form of the greens function and that the term so, the term in the right that is this term is equal to nothing, but equal to minus G a k tau plus beta for we have taken that from 0 less than tau less than or rather minus beta less than minus beta less than tau less than 0. And so, this is the property that we were talking about and so, this equality is satisfied by as the same equality was satisfied by the function the arbitrary function that we had talked about.

And the, I this above identity this allows the greens function to be expanded in a Fourier series of the type.

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$$\mathcal{G}(k, i\omega_n) = \int_0^{\beta} d\tau\, e^{i\omega_n \tau}\, \mathcal{G}(k, \tau)$$

$$\mathcal{G}(k, \tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau}\, \mathcal{G}(k, i\omega_n)$$

$i\omega_n$ are odd multiples of π/β.

That G of k i omega n equal to 0 to beta d tau exponential i omega n tau and G k tau and the G k tau is written as 1 over beta sum over n, exponential minus i omega n tau and k i omega n. So, these properties are exactly save as that arbitrary function with omega n to the odd multiples of pi over beta.

So, your i omega n are odd multiples of pi over beta. So, this is formally representing the greens function the Matsubara greens function will do some examples with this and let us do 1 example and it is right down example.

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Example

Non-interacting Matsubara Green's function.

$$H = H_0 = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} \; ; \; K = K_0 = H_0 - \mu N = \sum_{k,\sigma} \xi_k c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$\xi_k = \epsilon_k - \mu .$$

τ evolution of the operators,

$$c_{k\sigma}(\tau) = e^{\tau K_0} c_{k\sigma} e^{-\tau K_0} = e^{-\xi_k \tau} c_{k\sigma}$$

$$c^{\dagger}_{k\sigma}(\tau) = e^{\tau K_0} c^{\dagger}_{k\sigma} e^{-\tau K_0} = e^{\xi_k \tau} c^{\dagger}_{k\sigma}$$

Baker - Haudorff Theorem

$$e^{A} c e^{-A} = c + [A, c] + \frac{1}{2!}[A,[A,c]] + \frac{1}{3!}[A,[A,[A,c]]] + \ldots$$

So, we write down the non-interacting greens function Matsubara greens function non interacting Matsubara greens function ok.

So, H H equal to H 0 which is equal to sum over k epsilon k C k sigma dagger C k sigma. Now here k is same as k 0 which is same as H 0 minus mu n, which is a k and a sigma and we have a xi a k C k xi k C k sigma dagger C k sigma where the xi k is nothing, but epsilon k minus mu. So, the tau evolution of the operators can be written as is that the C k sigma tau it is equal to exponential k 0 tau k 0 and the C k sigma exponential minus tau k 0 we just proved this in a while and this is equal to minus xi k tau C k sigma.

So, this is the tau evolution tau is remember tau is complex time. So, the tau tau evolutions of these are like this and similarly the tau evolution of the creation operator is like this.

And this can be proved using what is called as the Baker Hausdorff Theorem, which says that exponential A C exponential minus A equal to C plus C plus A C plus 1 by 2 factorial A A C and 1 by 3 factorial A A A C and so on.

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$$e^{\tau K_0} c_{k\sigma} e^{-\tau K_0} = c_{k\sigma} + [\tau K_0, c_{k\sigma}] + \cdots \qquad K_0 = \sum_{k,\sigma} \xi_k c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$\tau \xi_k [c^{\dagger}_{k\sigma} c_{k\sigma}, c_{k\sigma}] = \tau \xi_k c_{k\sigma}$$

$$c_{k\sigma} = c_{k\sigma} - (\xi_k \tau) c_{k\sigma} + \frac{(\xi_k \tau)^2}{2!} c_{k\sigma} - \cdots$$

$$= e^{-\tau \xi_k} c_{k\sigma}$$

$$g^{(0)}(k,\tau) = -\Theta(\tau) e^{-\xi_k \tau} \langle c_{k\sigma} c^{\dagger}_{k\sigma} \rangle + \Theta(-\tau) e^{-\xi_k \tau} \langle c^{\dagger}_{k\sigma} c_{k\sigma} \rangle$$

$$= e^{-\xi_k \tau} \{ \Theta(\tau) [1 - n_F(\xi_k)] - \Theta(-\tau) n_F(\xi_k) \}$$

$$n_F(\xi_k) = \langle c^{\dagger}_{k\sigma} c_{k\sigma} \rangle = \frac{1}{e^{\beta \xi_k} + 1}$$

So, this can be applied to our case where we have an exponential tau k 0 C k sigma and exponential minus tau k 0 this can be written as C k sigma plus tau k 0 C k sigma and plus so on. And tau xi k which is k 0 is H H 0 minus omega n. So, k 0 is equal to sum over k xi k C k sigma dagger C k sigma where thus. So, this is a tau xi k will come out and I will have a C k sigma dagger C k sigma with C k sigma, which is simply equal to tau xi k C k C k sigma C k sigma.

And hence we can write down a C k sigma to be equal to C k sigma minus a xi k tau C k sigma plus a xi k tau square by 2 factorial C k sigma and so on. And this can be actually written down as an exponential tau xi k C k sigma and so on. So, that is how we can write down the greens function for the non-interacting problem, which for which I have introduced this 0 and this is written as a minus theta of tau an exponential minus xi k tau and a C k sigma dagger C k sigma and plus the other term theta tau exponential minus xi psi k tau C k sigma dagger C k C k sigma, we have written it somewhat sloppily it has to be here and so on.

And this can be written as exponential minus xi k tau and a theta tau 1 minus n F xi k we have shown that this is equal to this angular bracket is equal to 1 minus n F and theta of tau to be a minus tau to be here there is a minus tau here, which is n f xi of k. So, the the 2 combined so n F is nothing, but equal to n F of xi k is nothing, but a C k sigma dagger C k sigma, which is equal to 1 divided by exponential beta xi k plus 1. It is easy to obtain the frequency dependent greens function, which is equal to k and i omega n which is nothing, but a 0 to beta d tau exponential i omega n tau G 0.

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$$\mathcal{G}^{(0)}(k,i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\, \mathcal{G}^{(0)}(k,\tau) = -(1-n_F)\int_0^\beta d\tau\, e^{i\tau(\omega_n-\xi_k)}$$

$$= -\frac{(1-n_F)\left(e^{\beta(i\omega_n-\xi_k)}-1\right)^0}{i\omega_n-\xi_k}.$$

$$e^{i\beta\omega_n} = -1 \qquad i\beta n = (2n+1)i\pi$$

$$\mathcal{G}^{(0)}(k,i\omega_n) = \frac{(1-n_F)\left(e^{-\beta\xi_k}+1\right)}{i\omega_n-\xi_k} = \frac{1}{i\omega_n-\xi_k}$$

$$1-n_F = \frac{1}{e^{-\beta\xi_k}+1} \qquad i\omega_n \to \omega_n + i\eta.$$

And a k tau minus 1 minus n f 0 to beta d tau exponential i tau omega n minus xi k and this is written as 1 minus of 1 minus n F and exponential beta i omega n minus xi k minus 1 divided by i omega n minus xi k.

Remember that the second term in the numerator here can be simplified if we use exponential i beta omega n to be equal to minus 1 for i beta n to be 2 n plus 1 i pi, and then I can write down the greens function the zeroeth order greens function as k i omega n which is equal to 1 minus n F exponential beta minus beta xi k plus 1 divided by i omega n minus xi k it is equal to i omega n minus xi k, because my 1 minus n F equal to exponential minus beta xi k plus 1.

So, the temperature information is encoded in the frequencies omega n. So, now as we said that the 0 temperature result would be obtained by analytic continuation of i omega n going to omega n plus i eta to the real axis and in the and so, in the same spirit as the 0 temperature the minus the plus sign would relate it to retarded greens function and the minus sign would be an advanced greens function.

So, this is how the 0 temperature limit is taken from the finite temperature and the reason that the 0 temperature limit is relevant is that, because the benchmarking temperature scale in Fermionic system is given by the Fermi temperature. And the Fermi temperature for metals it is of the order of 70 80000 Kelvin.

So, even a temperature which is room temperature 300 Kelvin can be taken as 0 temperatures. So, sometimes in fermionic systems, we may need or we can get by with 0 temperature properties or 0 temperature formula that is relevant even when the temperature of the system is or the experiments are done at room temperature.