Advanced Condensed Matter Physics
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Lecture – 17
Dyson's equation and disorder in electronic systems

So, let us do the Dyson's equation for the Matsubara greens functions.

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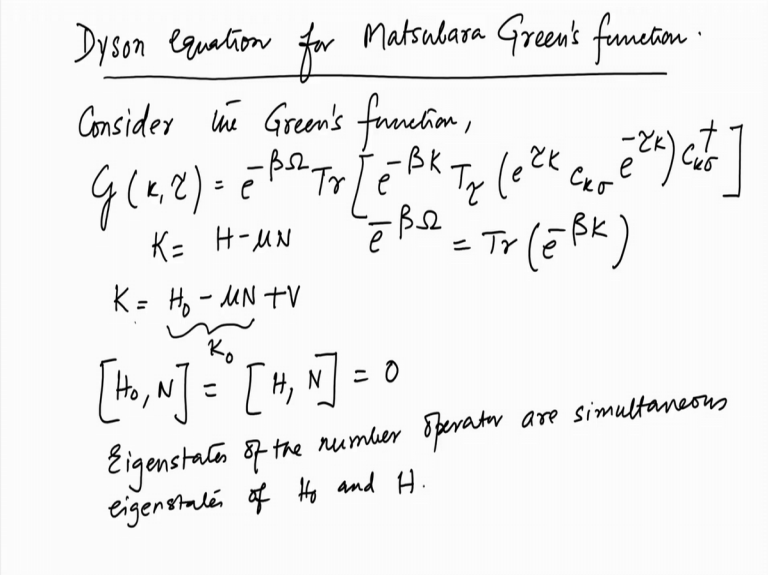

So, this is in line with what we have done for the 0 temperature greens function. So, from the discussion so, far it is evident that the Matsubara greens function formerly looks similar to that 0 temperature greens functions.

Excepting that, now we are talking about a complex time being bounded by minus beta 2 plus beta, and the information about the temperature enters through the quantization of the frequencies. And in case of fermions the frequencies are quantized in odd multiples of pi over beta and for the bosons they are quantized in terms of even multiples of pi over beta.

So, we need to now write down a Dyson's equation in which we want to avoid doing a finite order perturbation theory and want to invoke all orders of H prime into the sum and we have seen that this is quite a doable exercise.

So, consider the greens function G k the keys are vectors, but since we have not been putting. So, let us just remove this and t tau is what we have seen it is a minus beta omega and then there is a tress exponential minus beta k the tau an exponential tau k see k sigma exponential minus tau k C sigma dagger and that is that is the expression for the Matsubara greens function H to remind you that we are writing it with a calligraphic G omega is the grand potential.

And K is given by K is given by H minus mu N and exponential minus beta omega is equal to trace of exponential minus beta K. So, this is something that we have seen and K equal to H 0 minus mu N plus V, where V is the potential which typically represents a 2 body interaction term say it can represent an electron electron interaction of the coulomb, type which is what we have been most familiar with. So, now, so, the K 0 problem that is this part has already been solved. So, this is the K 0.

So, suppose we have been able to solve this exactly that is without the interaction term it is been solved exactly. And also that our these H 0 commutes with the number operator and so, does the total H which includes H naught plus V with the number operator that commutes. And so, the eigenstates of eigenstates of the number operator are simultaneous eigenstates of both H 0 and H. So, let us write down the operators in the interaction representation.

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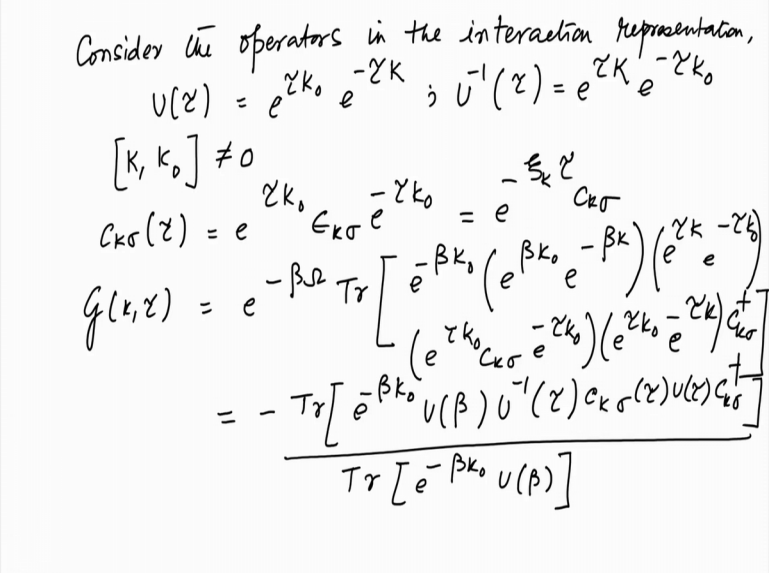

And write those unitary operators which we have introduced earlier, but with real time as exponential tau K 0 and exponential tau K if you remember that we have written down similar operators with I T and with H 0 and so, this is not H, but I will write it as k. We had written it earlier for the 0 temperature problem with tau as I T and k 0's as H 0 and k as H and so on.

Similarly we would have a u inverse tau which is equal to exponential tau K exponential tau K 0 needless to say that K and K 0 do not commute, I mean rather there is a part of K 0 which does not commute there is a part of K which does not come out with K 0.

So, as we have written it earlier the operators can be written as C k sigma tau which is equal to exponential tau k 0 epsilon k sigma exponential minus tau k 0, which is equal to exponential xi k tau and the C k sigma this has been proved earlier that is the tau evolution of the or the imaginary time evolution of the operators.

And hence we can put them into the this G k tau which is equal to exponential minus beta omega. And then a trace of exponential minus beta k 0 we have just introduced, exponential beta k 0 exponential minus beta k. So, we have introduced this exponential minus beta 0 and exponential plus beta 0. And then exponential tau k exponential minus tau k 0 and again we have exponential tau k 0 C k sigma exponential minus tau k 0 exponential tau k 0 exponential minus tau k and C k sigma dagger that is our greens function.

And this can be written as this can be written as we have a minus stress of exponential minus beta k 0 u of beta, see the definition of u here it is exponential tau k 0 and exponential minus tau k. So, that is written here as u of beta. So, the whole idea of writing it into this then this particular form is to introduce this u operators and then you have a u inverse tau and C k sigma tau and a u tau and C case sigma dagger and this is divided by trace of exponential minus beta k 0 u of beta.

Ah just show in a moment that how this thing comes.

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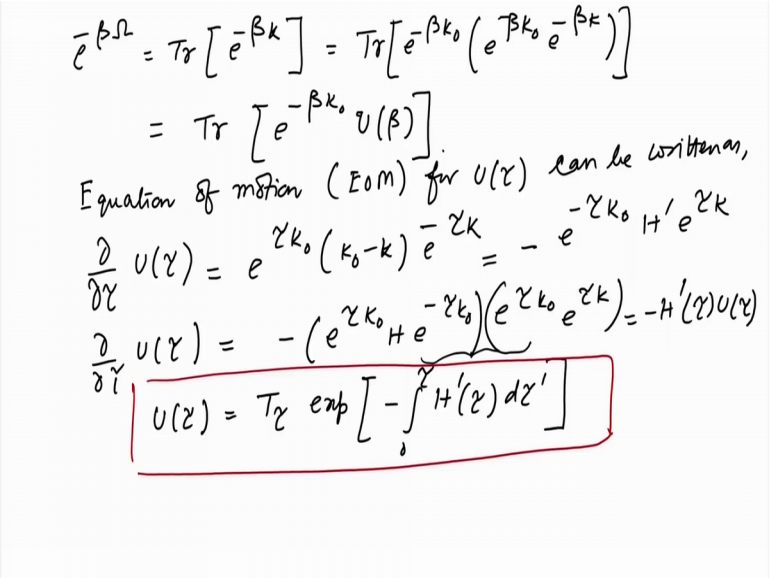

So, we have u exponential minus beta omega that can be written as trace of exponential minus beta k and now I will introduce this factor of exponential beta k 0 and exponential minus beta k 0. So, this is stress of exponential minus beta k 0 and exponential beta k 0 exponential minus beta k and this is equal to trace of trace of exponential minus beta k 0 u of beta.

So, a similar substitution can also be has also been made in the numerator for the exponential minus beta k and that is how this exponential minus beta omega is replaced by trace of exponential minus beta k 0 u of beta in the denominator. So, the equation of motion, which in short will call as EOM can be for u of eta can be written as del del tau u of tau will have 2 there are 2 factors in u consisting of exponential tau k 0 and exponential minus tau k.

So, one has to be kept constant the other will be differentiated and vice versa will have to be done and in which case we can write this as exponential tau k 0 with a k 0 minus k exponential minus tau k and we know k 0 minus k is nothing, but it is equal to minus of H prime and this is equal to minus of exponential tau k 0 H prime exponential tau k. So, del del del del tau of u tau which is the precisely the equation of motion can be written as exponential tau k 0 H prime exponential tau k 0, exponential tau k 0 and exponential tau k.

So, this part has been introduced and such that we can write this as a minus H prime T sorry not T, but this will be tau this tau and u of tau. So, so we have seen this kind of an equation, we can write down the equation of this differential or the solution of this differential equation as t tau exponential minus 0 to tau H prime tau d tau prime.

So, this is the solution of the unitary operator that we have introduced and all these discussions are simply complementary to the 2 the ones that we have done for T equal to 0.

So, this is the solution for u of tau.

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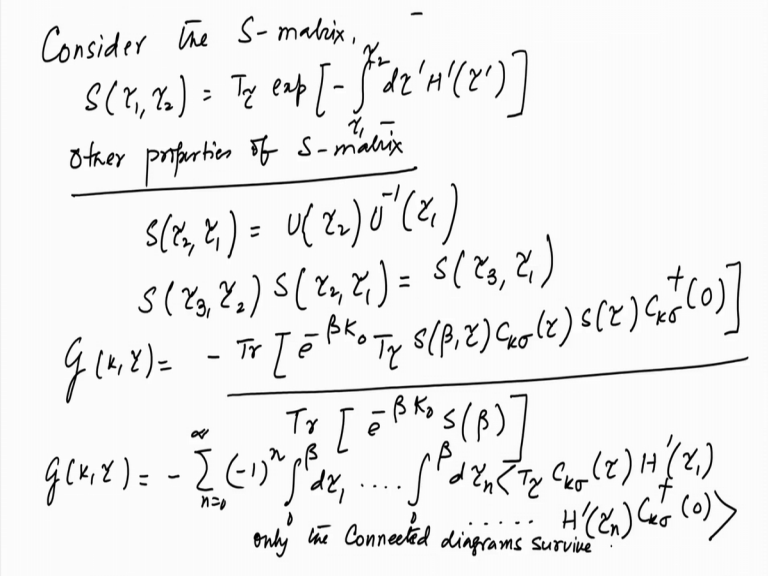

Similarly we can write it for the S matrix S tau 1 tau 2 equal to T tau exponential minus tau 1, tau 2 d tau prime H prime tau prime. So, that is the definition of S matrix other properties of S matrix that includes that S tau 2 tau 1 can be written in terms of the U operators like u inverse tau 1.

And also the tau 3 tau 2 and multiplied by tau 2 tau 1 will combine to give tau 3 tau 1 all these properties we have seen for the S matrix. So, with all these inputs we can write down the greens function as k tau this is equal to minus trace of exponential minus beta k 0 T tau S beta tau C k sigma tau S tau C k sigma dagger tau and sorry this will be 0.

And, that the denominator comprising of exponential minus beta k 0 S of beta and so on. So, at the end what is going to happen is that the disconnected diagrams as we have seen

are going to cancel with the denominator and will be left with only the numerator and in which case the G k tau is equal to a minus n equal to 0 to infinity minus one whole to the power n 0 to beta d tau one and so on 0 to beta d tau n and we have a T tau C k sigma tau H prime tau 1.

And all the way till H prime n C k sigma dagger 0. So, that angular bracket is closing. So, this is the expression for the full greens function including all the all orders of the interaction term H prime. As we told that the H prime could be of the coulomb type or for that matter any other type and we are uncommitted about the nature of the interaction, but if there is an interaction electron electron interaction in the system the full greens function Matsubara greens function will be like this where as u n equal to 0 will be the 0th order 0 and 1 will be till the first order and so on. So, we can take do a perturbation theory in terms of H prime and can write down a greens function to a particular order that is desirable to us.

Now, the question is that if for a given problem doing a perturbation theory up to a given order is not a satisfactory treatment of the problem. It could happen that there are suppose one takes care up to second order of H prime, and then it turns out that the H third order is equally important as the second order and the fourth order could be as important or at least halfway as important as the third order and so on.

In which case we have to go to higher orders and in principle we have to include all orders of H prime and write down a like equation and this is what we are planning to do here.

So, just to say that in this particular things only the connected diagrams survive all right.

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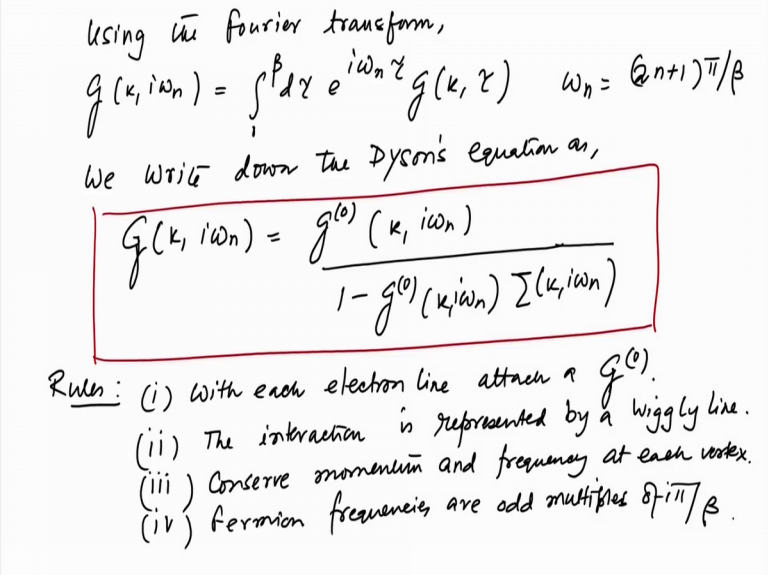

So, now using the Fourier transform G k i omega n this is equal to 0 to beta d tau and exponential i omega n tau and G k tau. So, will use this Fourier transform and of course, knowing fully well that my omega n is 2 n plus 1 pi over beta. So, that is the how the frequencies are quantized in odd multiples of pi over beta.

So, we write down Dyson's equation as G k i omega n this is now we do a Fourier transform of this and then this is written as G 0 k i omega n divided by 1 minus G 0 k i omega n and the sigma k i omega n. So, it is exactly a similar expression we have seen which we have derived for the 0 temperature greens function.

Sigma being the self-energy and for a particular case we have also seen how to compute the self-energy all these rules of writing down the diagrams or rather you know sketching down the diagrams and getting out information about the scattering process follows exactly in the same manner that we have seen. So, the rules just to give you once again the rules is that with each electron line attached G 0 the interaction interaction is represented by a wiggly line.

Conserve momentum and frequency at each vertex and also do not forget that the fermion frequencies are odd multiples of pi by beta whereas, the for boson frequencies are even multiples of pi by beta or we can write it as i pi by beta.

So, having done this formally let us try to do 1 example with the Matsubara function and see that how it enriches our understanding of problems in condensed matter physics? In principle disorder or defects is indispensable in condensed matter systems. So, these are

necessarily present and even if 1 tries to make an ultra-clean sample these are always there and they constantly affect the experimental results depending on the degree at which they are present. Sometimes they are necessary like in quantum hall effect they are absolutely necessary to have the hall plateaus to be quantized either in integer or in some chosen rational fraction of the quantity e square over H.

And sometimes they are non-desirable altogether in any case will do an example of this kind, but before that let us do the equation of motion of the Matsubara greens function.

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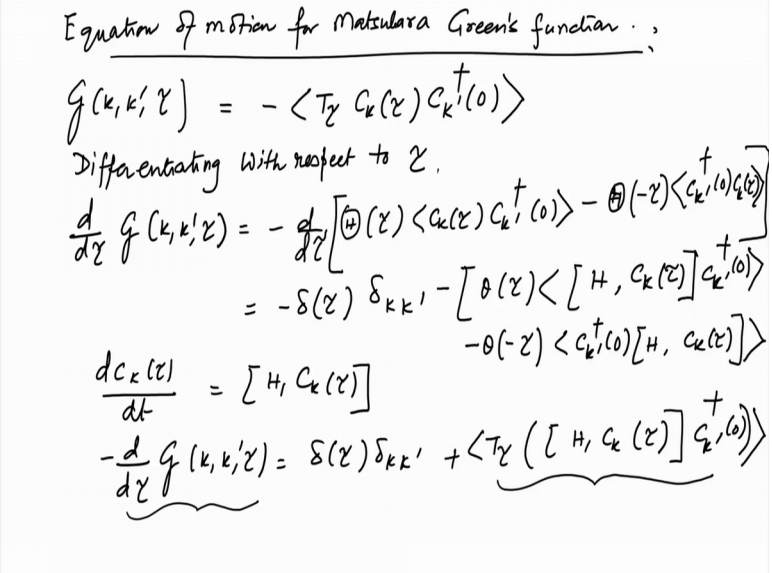

all right. So, we can we can take this k k prime and tau we can we can keep 1 index for the momentum or we can keep 2 indices it does not matter, let us just for generality let us take 2 indices and these are T tau C k tau just dropping the spin index for the moment 1 can put it back and a C k dagger 0 C k prime dagger 0 and the angular bracket closes here. Now differentiating with respect to tau we have so, d d T equal to a minus d d T of.

Now, this time ordering as we know that can be easily replaced by the theta function. So, will do that theta of tau C k tau C k prime daggers 0 and minus theta of tau, we have been writing it as capital theta let us write it a little neatly here and of minus tau and we have a C k prime dagger 0 C k tau this thing closes and the bracket closes is well. So, this is this is these are the 2 terms.

Now, to remind you that the derivative. So, this is not d d T this is d d tau and the derivative of a theta function is a delta function. So, we have a minus delta tau delta k k prime, now that comes because delta tau gives me tau equal to 0 in which they become equal time greens function.

So, they will have to have delta k k prime otherwise this angular bracket will become equal to 0 this is all what we have learnt, when we were dealing with fermion operators minus theta of tau and these are I am writing down for the time derivative to be in terms of the equation of motion of each of the operators, which are H this C k tau C k tau and a C k prime dagger 0 this and then there will be a term which is minus theta of minus tau and this we have a C k prime dagger 0 and H C k tau and so on.

So, we have used d C k tau d T to be the equation of motion for which is H C k tau where H is the total Hamiltonian for the system including the there is H 0 and v.

We have not taken for no particular reason though we have not taken the k here, but we could you could just write down k instead of H without any difficulty. So, minus i so, there are 2 minus signs. So, we will absorb that and write down the left the left hand side with a minus sign. So, this is k k prime tau it is equal to delta tau delta k k prime plus a T tau H C k tau C k prime dagger 0 0 and this with another bracket closing here let me just do it.

So, the important thing is that if H or k for that matter contains interaction term as coulomb term ok, which is a 4 operator term or a 2 body term and then this side that is this one will involve. So, H contains a 4 operator term and we are taking commutation with C k. So, this will involve higher order greens functions such as 2 particle greens function. So, when you try to write down the equation of motion for 2 particle greens function here, it goes and demands that knowledge of a larger particle greens function that is a 3 part of the greens function etcetera that should be available.

And then a 3 particle the equation of motion for a 3 part of the greens function would require even higher particle greens function. However, there is a way to terminate that series we are not going to discuss that here, for our case it is sufficient to talk about that let us suppose.

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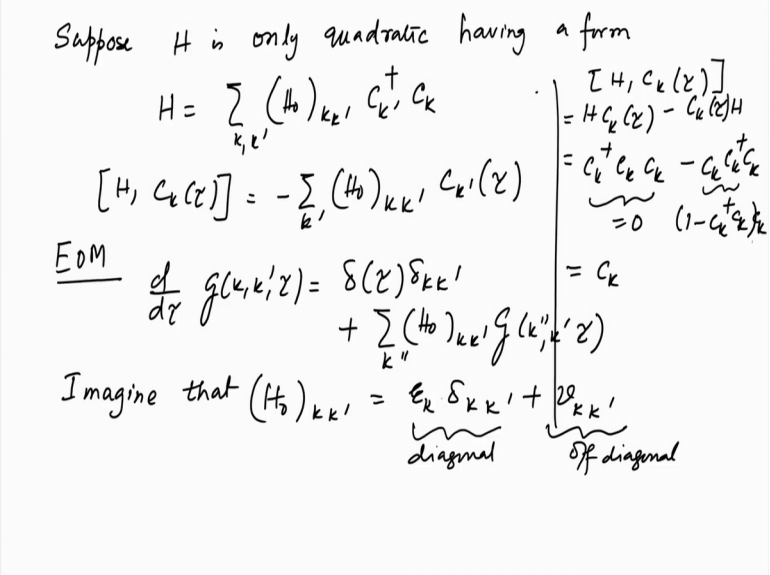

H is only quadratic having a form. So, we are not talking about interaction terms immediately let us just start with the free particle once. So, it is quadratic in electron operators and it has a form which is H equal to sum over k k prime and H 0 k k prime C k prime dagger C k C k.

So, this gives that the H acting on C k tau gives me that minus k prime H 0 k k prime and a C k prime tau, that is the that is what is given by the commutation of H with C k tau which you can chec k easily let us do that here. So, H C k tau minus C k tau h so, this is the meaning of H and C k tau.

So, this is equal to secret tau H and this is equal to this is equal to C k dagger C k C k and a C k C k dagger C k that kind of a term and of course, this is equal to 0, because there are 2 annihilation operators while 1 can write this down change the order and write it as 1 minus C k dagger C k C k C k. So, C k will multiply with 1 and give me a C k and again seek a dagger C k C k will give me 0 and this will give me a simple C k and that is what is written there. So, the equation of motion yields.

So, will write it as u M as a as an abbreviation for the equation of motion. So, the equation of motion is d d tau of G k k prime tau, which is equal to delta tau delta k k prime plus sum over k double prime H 0 k k prime G k prime k double prime k prime and tau. So, that is the form of the greens function of the equation of motion of the greens function, the first term contains just the delta function which is operative at tau

equal to 0 and it is a diagonal terms that if k becomes equal to does not become equal to k prime, then that term cancels out and the other 1 is the off diagonal term.

Now, let us imagine that H 0 k k prime contains diagonal part which is epsilon k delta k k prime and plus an off diagonal part, which is given by v k k prime which means this is the diagonal term and this is the off diagonal term. Why we are doing this we want to see the disorder effects, which would be included through the second term which is of diagonal and the kinetic energy is actually the diagonal term.

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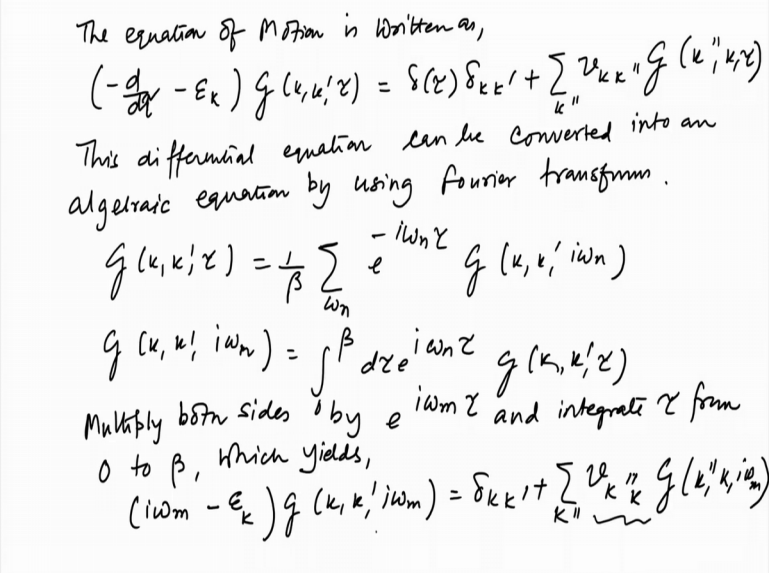

Now, the equation of motion is written as minus d d T or rather tau minus xi k and k k prime tau, this is equal to delta tau delta k k prime and plus v k k double prime and G k prime k tau. So, that is the equation of motion for the Hamiltonian to have a diagonal term as well as an off diagonal term as I told the diagonal term corresponds to say operators such as kinetic energy whereas, the off diagonal terms can denote quantities such a disorder or defects in the problem.

So, this is my equation of motion now this differential equation can be converted into an algebraic equation into an algebraic equation by using Fourier transforms and what do I mean by that that is so, I have G k k prime tau it is equal to 1 over beta sum over omega n exponential minus omega n tau and a G k k prime i omega n.

So, this is the the Fourier transform that we have and the inverse Fourier transform is k k prime i omega n equal to 0 to beta d tau exponential i omega n tau G k k prime tau.

So, you see the G k k prime tau is has a Fourier transform in terms of the G k k prime i omega n omega n 2 pi n i pi over beta. So, now, what we can do is that we multiply both sides multiply both sides by exponential i omega m tau and integrate tau, from 0 to beta which yields i omega m minus xi k or it could be here as we have not introduced the mu explicitly we can write it as epsilon k, G k k prime i omega m equal to delta k k primed as the first term. And there is a second term which consists of the off diagonal terms which is v k double prime k and G k double prime k prime i omega m.

So, that is what comes when you multiply it by exponential i omega m tau and integrate from 0 to beta and then we have used here.

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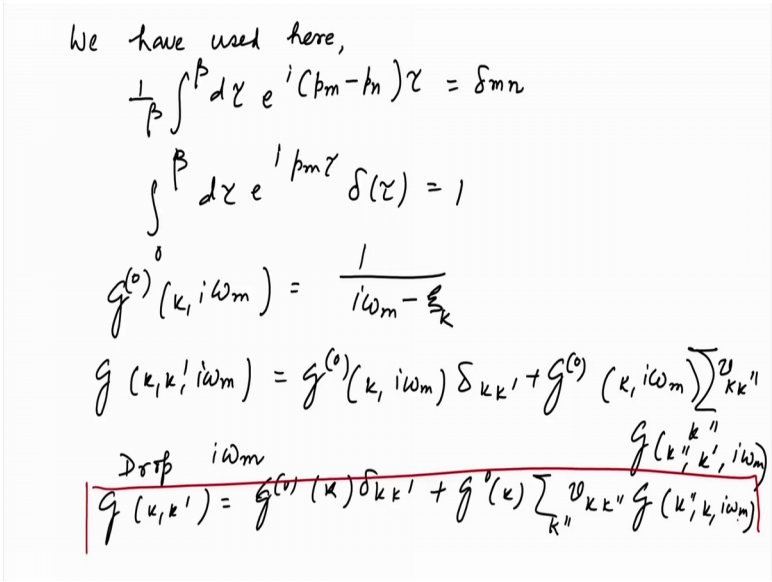

G 0, rather we have used 1 over beta 0 to beta d tau exponential i p m minus p n tau equal to delta m n and exponential beta d tau exponential i p m tau delta tau which is equal to 1.

Now, we know that G 0 k i p m which is here we are writing it as omega m equal to i omega m minus xi k. So, then the full greens function is written as G k k prime i omega m equal to G 0 k i omega m delta k k prime plus G 0 k i omega i omega m.

Ah And there is a sum over k double prime and there is there is a v k k double prime and there is a G k double prime k 1 i omega m there is a sum over. So, there is a k double prime and the k i prime. So, this is the form of the greens function when we have the Hamiltonian contains a term which is diagonal in k and there is also an off diagonal terms in k.

Though we are saying k we really mean any quantum numbers which is suitable for the which forms suitable basis for the problem will have. So, there could be a lambda and lambda prime in principle, which would the calculation would go through exactly. Now you see that both the sides depend on i omega m since both sides depend on a single variable at. So, at that at a particular value of the variable they will all i mean this equation will be valid.

So, that tells that I can actually drop i omega m it is not required to keep it. So, in both the sides and we can write down this as an infinite series. So, drop i omega m and write down G k k prime equal to G 0 k delta k k prime plus G 0 k v k k prime k k double prime G 0 k prime k i omega m.

So, that is the greens function that we write.

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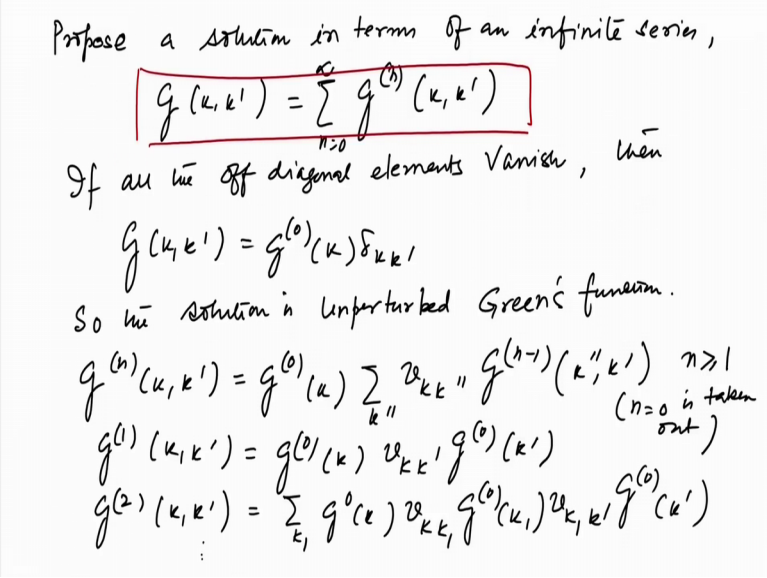

we can propose a solution of the type in terms of an infinite series and which is of the form that G k k prime equal to sum over n equal to 0 to infinity G n k k prime.

And so, if all the off diagonal elements vanish so, this is the first approximation if all the off diagonal elements vanish. Then we have the G k k prime equal to G 0 k delta k k prime. So, when we have no of diagonal elements only diagonal elements the solution of the greens function is purely the unperturbed greens function so the solution.

So, now if we insert this solution that we have written here into the equation that is here. So, if we insert 1 into another, then we can iterate the solution and take out the zeroeth order because we have already written the zeroeth order. So, H a G a G n k k prime equal to a G 0 so, this is the full solution I am writing it down it is k and then there is a k double prime v k k prime G n minus 1 k prime k k double prime k prime and this is for n greater than equal to 1.

So, n equal to 0 is taken out. So, if we iterate this then what we get is the following. So, the first order k k prime equal to G 0 and k and a v k k prime G 0 k prime. And a G 2 k k prime equal to a sum over k 1 G 0 k v k k 1 v is the the term that we have taken as the off diagonal term here.

So, v k k 1 there is a G 0 k 1 v k 1 k prime G 0 k prime and so on. There will be G 2 and G 3 and so on.

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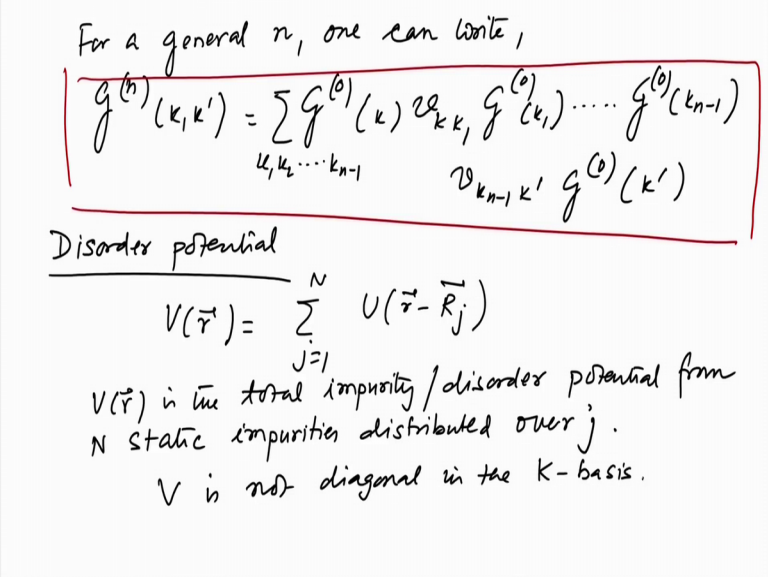

So, for a general n, one can write G n k k prime equal to k 1 k 2 and all that excepting the k will reserve. So, these are all will be summed over and there is a G 0 k then there is a v

k k 1 G 0 k 1 and going all the way up to all these G zeroes k n minus 1 v k n minus 1 and k prime and now you have a G 0 k prime.

So, at the order we are simply able to write this as n non interacting greens function. So, that which are solvable or which can be found out or we have already found them out which is like i omega m minus i k so, all these things. So, depends on which order 1 once one can find out this greens function till the order, if you want it till the first order or the second order you simply need to plug in this v k k 1 or v k k 2, whichever the diagonal terms are and these are the non-interacting greens function which we have already have learned how to write them.

So, this is the pretty much the solution for this problem in which we are simply talking about still not talking about the interaction term, but talking about the Hamiltonian being quadratic in terms of the operators, what are these calculations good for let us apply them to a disorder potential.

So, what it means is that at every lattice site there is a potential which could be randomly varying from 1 lattice site to another lattice site. So, and which are which could be purely random or which could be correlated, but this denotes an extra bit of potential at each lattice site and this could be written as a v of R, which is equal to sum over j 1 to n U R minus R j. So, what we did is that we have taken u to be the potential and there are j of j such disorder sites where the potentials are present. So, which are given by all these are R u R minus R j and then when we sum over all these n sites which have all these disorder potentials we get the total disorder potential which is given by v of R.

So, v of R is the is the total impurity potential impurity or disorder whatever you want to call it since we are talking about discrete lattice sites. So, it is a impurity is a more appropriate word in this context from n static impurities distributed over G. So, clearly V is not diagonal in the k basis ok.

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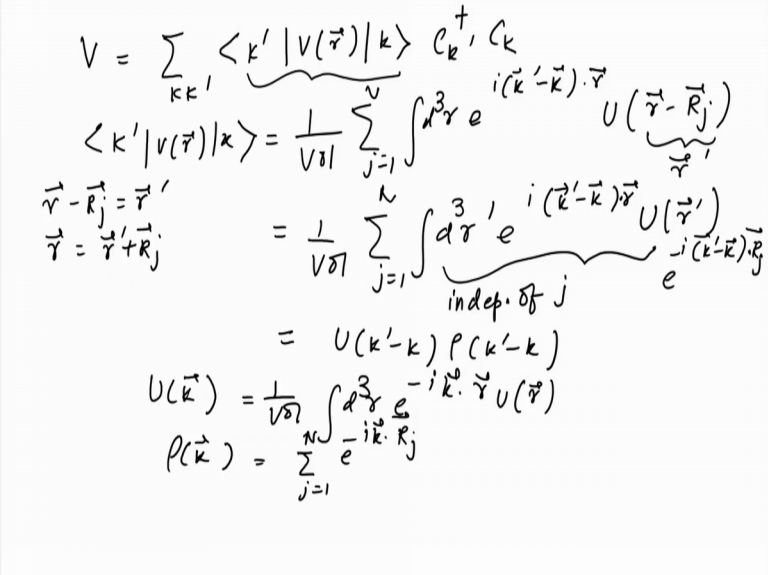

And how do we know that we can write down V which is equal to a k k prime a k prime v of r k and this would give me a C k dagger C k prime dagger C k. So, this is the kind of potential that we were talking about in our previous discussion when we spoke about off diagonal term in the Hamiltonian it is still non interacting, but there is an off diagonal term in the Hamiltonian which is something similar to that.

So, what is this matrix element this matrix element is given by k prime v of r k now there will be when you convert this expectation into integrations will have. So, 1 over volume will have to normalize it with the volume and there are n such impurities and we are say talking about 3 dimensions.

In principle we can talk about d dimensions here. So, it is a d cube r and an exponential i k prime minus k now will have to all put the vectors there because it is a product there so, U r minus R j and. So, let us assume that this is equal to a dummy r prime. So, if r equal r minus R j is equal to r prime r becomes equal to r prime plus R j and then this becomes equal to 1 by volume sum over j from 1 to n d cube r prime and exponential i k prime minus k r.

You just removing the vector signs knowing fully well that let us put this just to have completeness and U of U of r prime and an exponential exponential minus i k prime minus k dot R j where R j are the impurity sites. This is of course, you see that this is independent of j, which means the impurity sites and we can simply write this as you k prime minus k rho k prime minus k where U of k is equal to 1 over volume and d cube r

1 minus i k dot r u of r. So, this is the Fourier transform of these impurity potential and rho of k, which is simply equal to a sum over j equal to 1 to n exponential minus i k dot R j which gives the concentration or the density of the impurity.

So, it is clear that.

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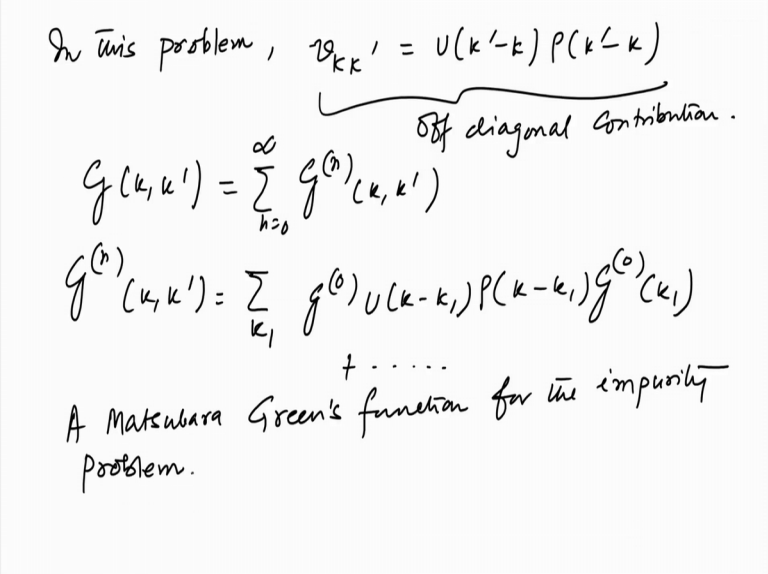

That in this problem in this problem we have a v k k prime equal to u k minus k prime minus k rho k prime minus k, which is the off diagonal contribution. And in which case we have G k k prime which can be written as n equal to 0 to infinity just like what we have done before and k k prime that is a solution, and where G n k k prime that is the order can be written as sum over k 1 and a G 0 u k minus k 1 rho k minus k 1 G 0 k 1 and all that other terms with k 2 for the second order and for the third order and so on.

So, one can iterate the solution , but in the first order this is the contribution coming from the off diagonal term which comes specifically from disorder. So, we have been able to write down a greens function or Matsubara Greens function function for the impurity problem ok.

So, this is one of the examples that we wanted to do for with the Matsubara greens function rest of the calculations as we have said exactly follows that of the T equal to 0, now the only difference being that there we have dealt with temperature and frequencies. Now here we would deal with complex time and complex rather frequencies, which are

having complex values and the temperature information actually enters through the frequency terms.