Dynamics of Classical and Quantum Fields: An Introduction

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Lattice Models
Lecture - 39
Schrieffer Wolff Transformation

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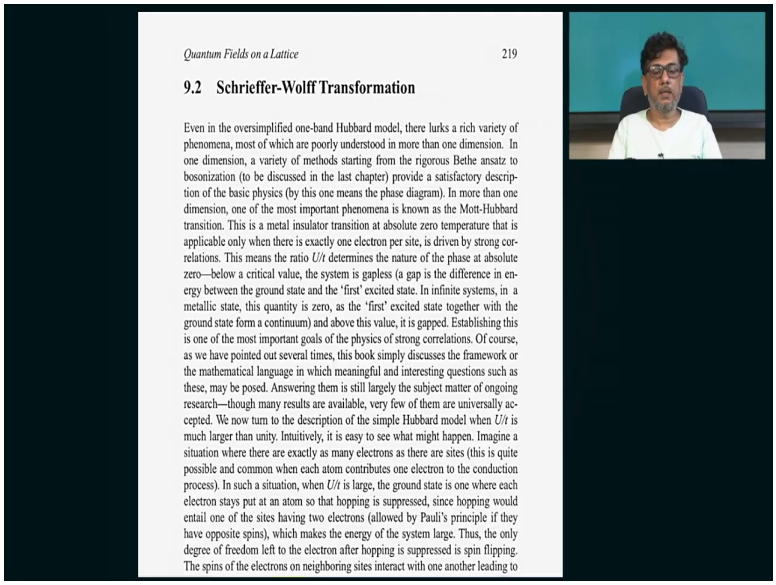

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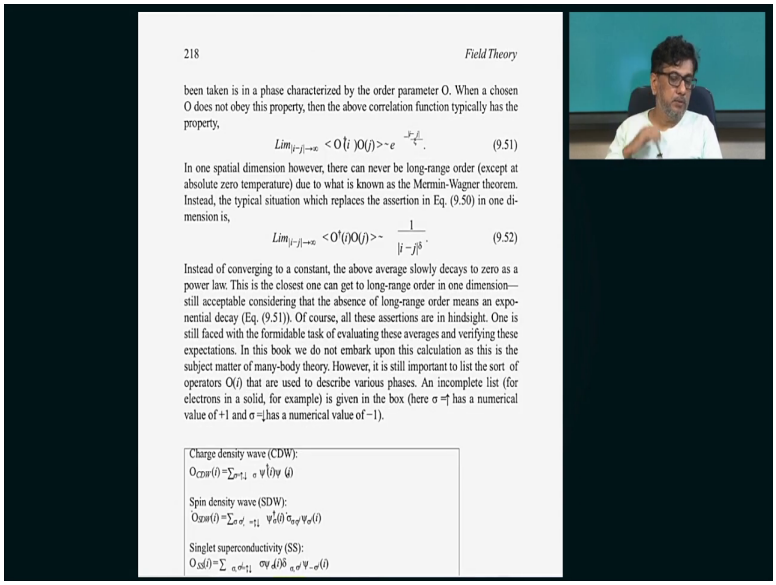

So, in this lecture, I am going to discuss a new topic which is the Schrieffer Wolff Transformation. So, if you remember in the last class, I had stopped at this stage where I pointed out that you can introduce certain operators called order parameters whose non zero, non vanishing, expectation value signifies the existence of various interesting phases.

So, in the next topic which will conclude this chapter will be the topic which explains to us how to transform this Hubbard model that we had encountered into a model that describes magnetism. So, you see magnetism is a kind of mystery especially ferromagnetism, if you think about it the fundamental basis for why there is ferromagnetism. After all if you imagine what ferromagnetism is.

It is basically a situation where you know you apply a magnetic field the material is magnetized that is easy to understand, but then if you remove the magnetic field, the magnetization does not go away. So, that is somewhat perplexing. So, it calls out for a fundamental explanation in terms of the behavior of the fundamental constituents of the substance.

So, that is something very not very obvious how to do that. So in fact, the way to do that is to invoke this type of an approach where we point out that if you start with this tight binding picture of electrons in a solid, there is a natural sense in which a magnetic insulator is obtained from that description. See, after all the Hubbard model includes very essentially two aspects one aspect is the hopping the kinetic term.

So, the electrons hop from one side to the other. So, that describes the conduction process or the bonding or whatever. So, whereas, the other aspect is the onsite coulomb repulsion. So, that is also there. So, there are two competing processes one process is the hopping, the other process the onsite repulsion. So, the ground state of the system is obtained by some kind of a compromise between these two competing processes. So, now, let us imagine a situation where you have precisely one electron per site.

So, that is not uncommon you might think that that might be very unusual and remarkable situation to have exactly one electron per site, but that is not in fact, it is very common because you can have a situation where exactly one electron an atom

contributes one electron to the conduction process. So, as a result you can you know the electrons that participate in the processes described in the Hubbard model are precisely one electron per side. So, imagine that is the situation that we are dealing with.

So, the point is that if there is one electron at a given site, the another electron can hop on to that site only if it suffers a coulomb repulsion; means, that there is an increase in energy due to the coulomb repulsion. So, the thing is that. So, if some site is left vacant that implies therefore, that some other site has two electrons in it. So, that is the implications of having precisely one electron per site.

So, that is called half filling. So, half filling because you see remember that an electron has up and down spin. So, a full filling would be having two electrons per site and that would be completely inert and uninteresting, because if you have two electrons per site what happens is that the electrons can I mean can do nothing, because they cannot hop because the already two electrons per site you cannot have three electrons per side.

So, you cannot hop ah, but then it can just, but those two electrons have to be one up one down, one up one down like that they have to be in pairs.

And they can do nothing but just stay there. They cannot even flip spins, because if they flip spins then they will be violating poly principle. So, that is absolutely uninteresting. So, the interesting situation is the half filling where you have one electron per site. So, where hopping is allowed, but at the cost of coulomb repulsion; that means, a mandatory cost of a coulomb repulsion because if you have less than half filling then you can hop around and many times you would not be suffering any penalty in terms of.

So, you can hop to an empty site and leave behind an empty site that is not an option when you have half filling. So, you have to hop around only at the expense of suffering a coulomb repulsion. So, that is the precise model that we are going to study ok. So, in this paragraph in this chapter, I have pointed out that even before you study the large repulsion limit of the Hubbard model, which I am going to study in this section, but there are very basic issues related to the Hubbard model.

One is something called the metal insulator transition. See, the idea is that if you have a Hubbard model and if the coulomb repulsion becomes large enough in more than in especially in three dimensions. So, you can show that the system goes from being a gapless system to a gapped system so; that means, it goes from being a metal to an insulator. So, the question is the one of the important goals in the study of Hubbard model is finding this critical value of u at which the system becomes an insulator from a metal.

So, these are all very difficult questions. And I told you that in this course, we will only be studying the models that are supposed to describe those type of phenomena. We would not be solving any of those models it is just meant to inform you that there are all these models that are worth solving. And when understood properly will are likely to exhibit these types of behavior ok.

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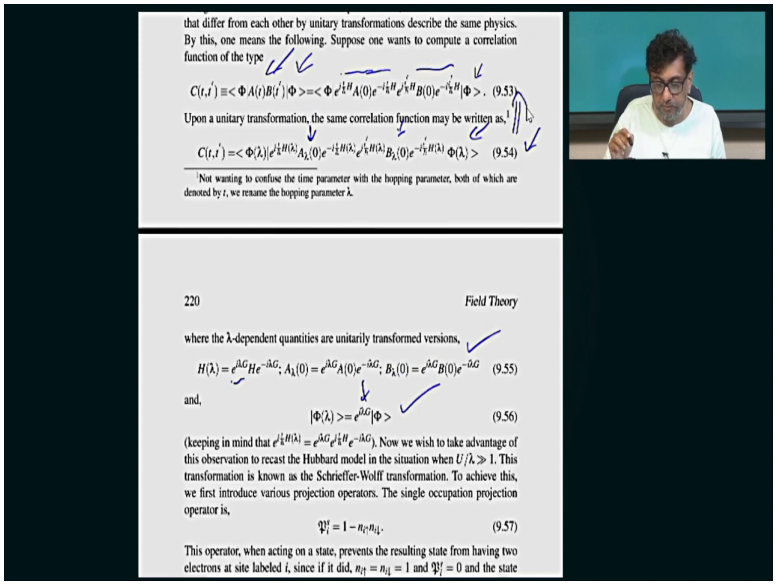

So, coming back to this large U limit. So, so the idea is that you see if you have half filling, if you have a model with exactly one electron per site. And you have a large U limit what; that means, is basically that the electrons will see on the one hand they would like to hop, but if they hop they will be suffering a coulomb repulsion. And if they suffer a coulomb repulsion and if that coulomb repression is progressively made larger and larger that becomes less and less attractive for the electrons to hop around.

So; that means, that given that there is a mandatory penalty of for hopping around namely the coulomb repulsion capital U. And if you make that larger and larger there is a it becomes less and less attractive for the electrons to hop. So, in the limit that U becomes very large. So, the electrons would prefer to stay put.

So; that means, you have precisely one electron per site and they are refusing to hop around, but you might think that is resembling the two electrons per site where they are anywhere going to stay put and there is no choice even if U is small they simply cannot hop, but here U is large and this also simply cannot hop.

So, you might think these two are the same situations, but they are not, because there is one thing the half filling electrons can do which the fully filled electrons cannot do. Namely, they can flip the spin so; that means, you see if you have one electron per site there is a spin degeneracy the up spin is pretty much the same you know if you think about it that there is a because there is no coulomb repulsion there is freedom for it to be up or down.

So, there is no other electron sitting on top of it. So, therefore, what happens is that there is this system of electrons they are all staying put at their lattice locations. And they are refusing to hop. So, therefore, they form an insulator so; that means, there is no conduction process completely suppressed. So, it is an insulator, but; however, the dynamics is through spin flips, because there is the only dynamics that survives.

The electrons flip spin. So, therefore, it constitutes a magnetic insulator. So, it exhibits some sort of magnetism where to see what sort of magnetism, but it certainly exhibits some intrinsic form of magnetism and it is an insulator.

So, let us see what sort of magnetism this sort of model exhibits? So, for that I have to perform as somewhat technical transformation to uncover the precise effective Hamiltonian that describes such a model. So, the Hubbard model itself it is not very convenient to study the large U limit, because you see when U is very large all it says is that ni up times ni down should be 0.

So; that means, double occupancy is suppressed that is all it says, but then it does not say how the electron behaves in the presence or in the when a double occupancy is strictly forbidden, how does the electron behave that is not clear. So in fact, if you think about it both the hopping is suppressed because it is half filling and double occupancy is suppressed because U is large. So, it seems like both the kinetic and potential energies are 0, I mean hopping its after all what is Hubbard model its hopping plus potential energy that capital U n i up ni down.

So, if hopping is suppressed the first one is 0, if ni up times ni down is strictly 0 then the second one is 0. So, that does not make any sense so; obviously, we have to perform a kind of a series expansion in inverse powers of U. So, that only that will make sense. So, in order to do that we have to make certain observations to start with. First is that if you have a Hamiltonian the physics of that system is equally well captured by another Hamiltonian which is related to the original one through a unitary transformation.

So, if you do not believe me here is an explicit demonstration of that fact. So, suppose you want to calculate say the average of some suppose you have an operator which. So, we are working in the Heisenberg picture so; that means, the operators change with time so; that means, imagine you have an operator A which is a function of time, and another operator B which is also a function of time. So, now, imagine that you want to find the average of A as a function of time as a function of t times B as a function of t dash.

You want to find the average with respect to some state ok. So, how does that look like? So; obviously, it looks like this so; that means, you first construct the appropriate time involved operators this way, and then you find the average. So, now, the claim is that you see these this particular average is also identical it is mathematically the same as doing the following. So, it is the same as first that you know unitarily transforming this Hamiltonian where some operator which depends on some continuous parameter called lambda.

And then, similarly unitarily transforming the, these you know initial time values of these operators A and B also through the same unitary transformation. And lastly, you know evolve the state that you are studying also by this unitary transform. So, if e raised

to i lambda G. And G is the generator of the unitary transformation, and this is the unitary operator, which implements the transformation then clearly you can it is just a mathematical identity for you to substitute 9.55 and 9.56 into 9.54. And verify that 9.54 is exactly going to reduce to 9.53 ok.

So, that is a trivial activity I am not going to do it. So, that observation is important because you see it enables me to now construct some unitarily transformed Hamiltonian to study my physics rather than the original Hamiltonian. Notice, that the original Hamiltonian was somewhat clumsy in the sense that it had the hopping and it had a coulomb term which was plus U times ni up times ni down. And that u was a multiplicative factor of ni up and ni down.

So, if U is large is a and it is in the numerator it is not very convenient to do any kind of expansion with it. So, if U is large and it comes in the denominator then it is convenient because you can expand in powers of 1 by U. So, that is the whole idea. So, I want to write down a unitary transformation. So, that in some sense that large U comes in the denominator rather than the numerator ok. So, how do I achieve all that? So, to do that I am going to first introduce something called the projection operator.

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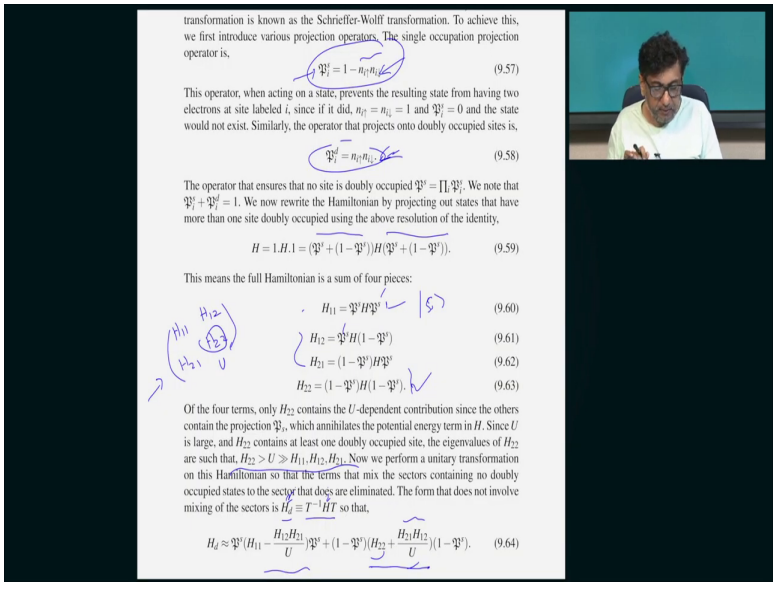

So, this projection operator is just defined like this. So, basically it says that the single occupancy projection operator. So, what it says is that it takes any state and if you act it on this projection operator it just destroys all the doubly occupied states.

So; that means, you see if you have a state you can express that in terms of you know no occupancy plus single occupancy plus double occupancy some kind of a linear combination like that. Now, if you take this operator and act it on that state it destroys the part of that state which contains the double occupancy.

And why is that because you see when there is double occupancy ni up times ni down will be 1 and 1 minus 1 is 0. So, basically it really suppresses the double occupancy part of that state. So, similarly the exact opposite of that is the one which weeds out the no I mean which weeds out everything except the double occupancy. So, that means, if any state has a single occupancy it kind of this type of projection operator weeds that out it only makes the double occupancy survive.

So, this makes the double occupancy survive, this makes only single occupancy survive or it also makes no occupancy survive, but that is not an option in the case we are considering because remember we are considering half filling where electrons are there is one electron per site and they are all staying put at their locations ok. So, bottom line is that I can always. So, this is a mathematical identity. So, I can this is just one written in afunny way. So, what I am going to do is that I am going to.

So, if I expand this out ill get four pieces. One is this H which has been sandwiched between two single occupancy projections. And there is one which has been sandwiched between a single occupancy, double occupancy projection. And lastly one which has been sandwiched between two double occupancy projections.

So, what this does is you see H 22 is the one that contains this, the contribution due to U. See because see the other operators will actually destroy any see these operators will all if you act it on any state the any double occupancy will immediately be destroyed by that.

So, this will destroy double occupancy. So, if you want to find matrix elements between states containing double occupancy. All these will be identically 0 except this one ok. So, this one will have the U dependent term. So, now, the idea is that the because only H 22 has the double occupancy U dependent term and U is very large. So, we are going to assume that H 22 therefore, is much larger than all the other three.

So; that means, H 22 is very large compared to H 11 H 1 H 2 1 and H 2 H 12. So, now, think of this as a kind of a matrix. So, you will see that it has a there is a deeper reason for why you can do that. So, think of it like this. So, now, you find the eigen values of. So, the claim is that the, you can write down a unitarily transformed Hamiltonian from H. So, you start with H and you write down a unitary transformation.

So, the claim is that the unitarily transformed Hamiltonian is going to have eigen values which correspond to the eigen values of this matrix. So, now, if you work this out and this is approximately U, ok.

So, if you work this out you will see that basically if when U is very large, the eigen values are precisely these two. So, you can just work this out. So, you will see that the Hamiltonian works out to be this and this. So, these will be the two eigen values.

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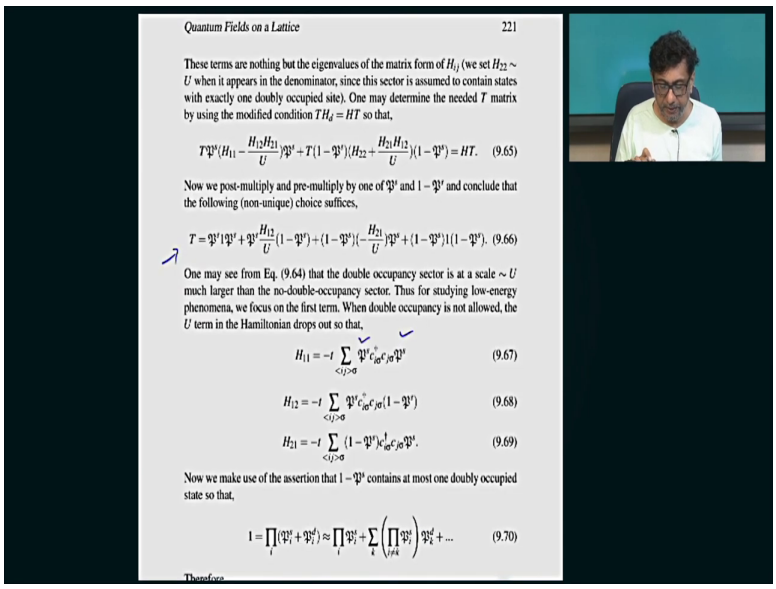

So, now you see if I know this seems rather ad hoc. So, the more systematic way of doing this is to say that look I am going to first postulate that there is a unitary operator called T of this sort.

So, then. So, if I use this T, then I can basically weed out all the double occupancy terms ok. So, I will end up with a term which is exceedingly small. So, the this one is any way of the order of U, the next correction will be of the order of 1 by U. So, I will end up making an expansion in powers of 1 by U ok. So, bottom line is that yeah. So, you will have to go through this these calculations in detail.

So, bottom line is that you see the H 11 is the hopping sandwich between the two single occupancy projections and so on and so forth. So, you have this H 12 which is a sandwich between single and double occupancy and so on and so forth.

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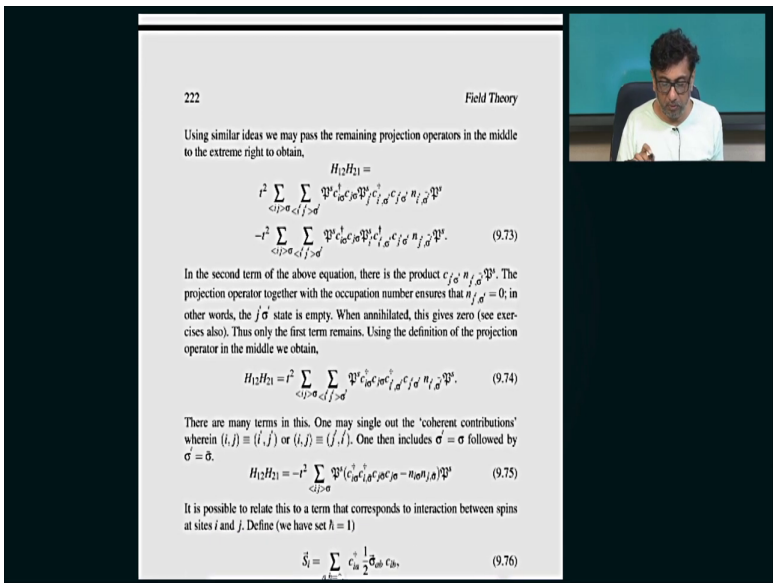

So, now you can go ahead and evaluate these types of products that appear in the in these expressions ok. So; that means, say here for example. So, when you do that. So, it is a lot of tedious algebra. So, I will have to request you to go through it. Because firstly, this proof is there in some review article and you would not be able to you will probably able to follow it with as much ease or difficulty as this particular lecture because the rest of the details are just a lot of tedious algebra.

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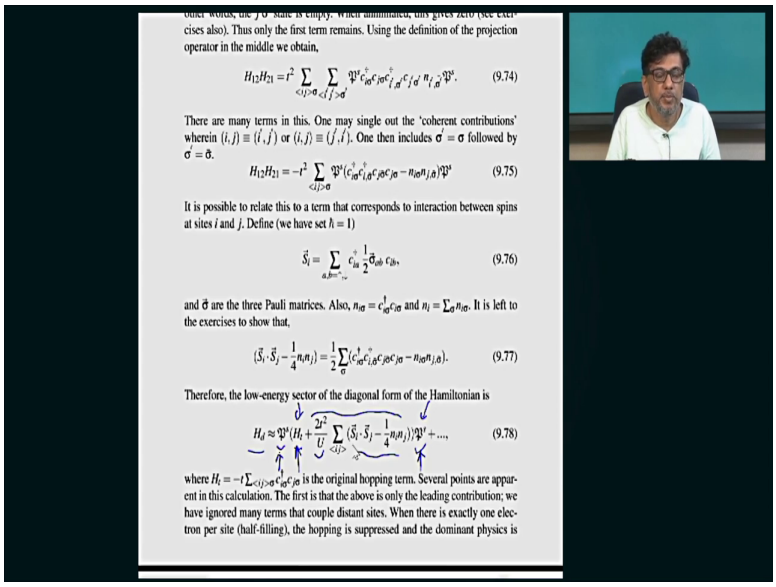

So, you just have to go through these algebra, and then you will see that finally, you will be able to write down a Hamiltonian which basically weeds out the.

So, what is the beta s again. So, beta s basically makes sure that if you have double occupancy it fully kills it; that means, if ni up plus ni down ni up times ni down is 1; that means, if there are two electrons in a site that beta s is 0. So, it makes sure that all the states are I mean basically it makes you that all states are singly occupied. So, therefore, the effective Hamiltonian of a system when you have a single electron per site.

And you have the coulomb repulsion between electrons is large the effective Hamiltonian involves hopping with the single occupancy means the hopping with the double occupancy fully suppressed because that is what beta s is. So, if there is a double occupancy beta s becomes 0. So, it does not allow double occupancy. So, what is H t? H t is your original hopping. So, basically your effective Hamiltonian is as if there is hopping, but then hopping subject to this constraint that you cannot have double occupancy on any site.

But, then there is an additional correction so; that means, that is that would be strictly true for infinite U. If U is actually infinite that will happen so; that means, you have a situation where infinite U Hubbard model. So, infinity U Hubbard model is same as just

hopping with the double occupancy is suppressed. So; that means, say you are not allowing double occupancy, but then remember that if you are strictly looking at half filled; that means, one electron per site then anyway hopping is suppressed because of that that reason.

So, therefore, this will identically be 0 in case of half filling. Half filling when you have large u and half filling hopping is anyway forbidden. So, if hopping is forbidden you cannot say the Hamiltonian is 0. So, there will be a leading term which corresponds to a magnetic insulator. So, I told you right. So, if you have a hopping is suppressed all that electrons can do is flip the spin sitting at their original locations. So, that is exactly what this term is telling you. So, this term tells you that there is a there is a mechanism there is a physical effect which is of the order of 1 by U, where the electrons flip spin.

So; that means, there is a spin spin interaction between nearest neighbors. So, the is nearest neighbor because remember the hopping. So, this somehow indirectly comes from hopping. So, it comes by diagonal I mean diagonalizing that unitary transformed matrix. So, basically there is a spin spin interaction that is induced by the fact by a kind of a conspiracy between the fact that you have single electron per site and a large repulsion. So, this is an example of a kind of magnetism. And this is in particular it is basically anti ferromagnetism.

Because U is positive and large T squared is positive. So, this is saying that energy is lowered if the neighboring spins are anti parallel. So; that means, one up one down one up one down. So, that sort of thing. So, this corresponds to a model of anti ferromagnetism ok. So, the point is that you see these lattice models are likely to give you various models of magnetism, if you know try to. So, the simplest Hubbard model gives you antiferromagnetism as a consequence of half filling and large U.

So, similarly there will be other models will which will give you other types of magnetism which we would not go into.

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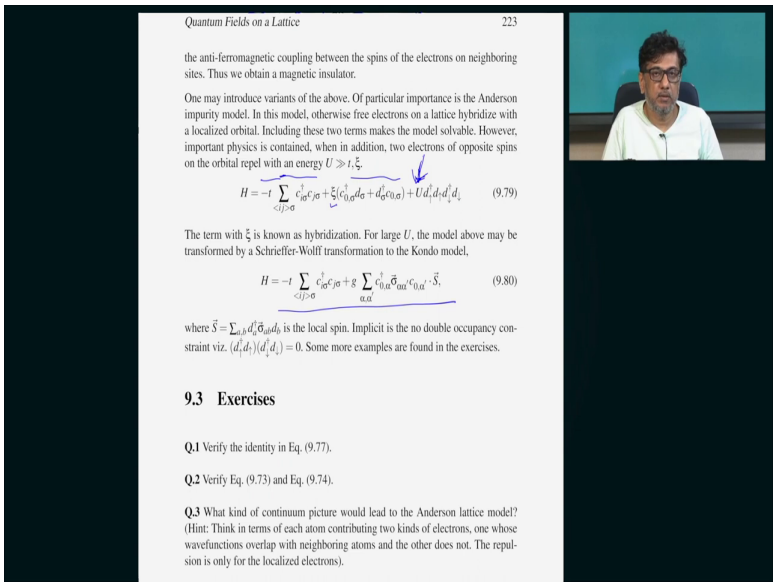

So, I will just stop this section with just pointing out that there is an interesting important model called the Kondo model. So, the Kondo models talks about a conduction electrons interacting with a localized quantum spin. So, the way that is thought of it may be thought of as the limiting case of a model with hybridization.

So; that means, so, imagine you have as usual a hopping situation. So, you have electrons which are itener and they are hopping. And there is a localized electron at some origin which is localized. And you can have two such electrons sitting on that localized site and corresponding to this coulomb repulsion, but then these electrons can hybridize with the localized electron so; that means, you can have a electron from this itinerant family of electrons to get transformed to this localized or the localized electrons can dislodge from the localized site and become itinerant.

So, bottom line is that you have this hybridization term. So, just like in the earlier example where the Hubbard model could have been transformed to a model involving magnetic moments. So, here to I can transform this you know hybridized model. So, it is called the Anderson single line impurity Anderson model. So, this can be transformed when U is very large to something called the Kondo model. So, the Kondo model describes the interaction of the itinerant spin of the electron with the localized spin that is sitting there ok.

So, this is a very important model in condensed matter, it has a important historical value also. So, similarly you can have a situation where you have a, Anderson lattice model so; that means, you have localized electrons sitting at various points in the lattice and then you have you know it itinerant electrons hybridizing with them. And the large U limit of that will give you something called the Kondo lattice model ok. So, that describes the behavior of conduction electrons interacting with a lattice of spins ok.

So, all these are important models in condensed matter physics. And I have just succeeded in maybe with some great effort. It might require persuasion, but I have somewhat succeeded in pointing out to you that it is possible to transform one into the other. You can transform a model which describes you know it inerrant electrons hybridizing with localized electrons into a model describing the interaction between the spins of the localized and the retainer and electrons, but the downside to this is that both are equally intractable.

So, all I have done is I have successfully mapped one unsolvable intractable problem into another perhaps even more intractable problem. So, in some sense it is not satisfying, because it does not it sheds some light in the sense that it if there is some inkling or some indication about where magnetism could come from some there is some indication that magnetism could come through these types of mechanisms in actual solids, but other than that there is absolutely no further information because I have not solved anything I have just pointed out all these models are interesting.

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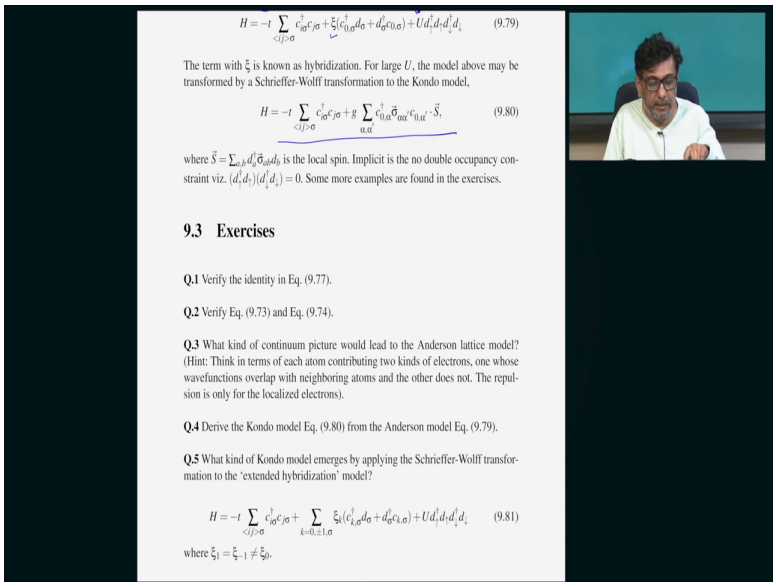

But unfortunately in this course that is the extent to which I can go. So, I will not be solving any model of any significance. I will simply be pointing out that such models are interesting and they are worth solving and that is for you to explore the research literature and find out more about them ok. So, I am going to stop here.

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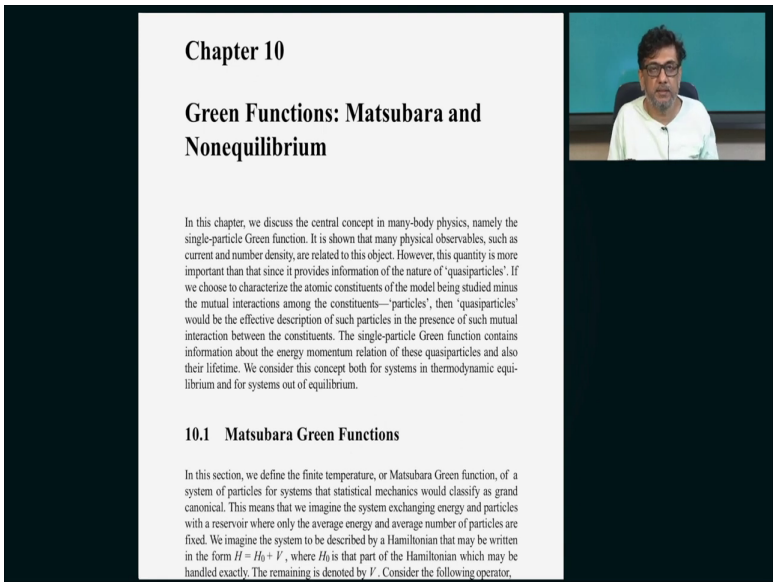

And in the next class, I will be discussing something slightly easier which is basically the idea of a finite temperature Green's function. So, if the system is in contact with some

thermal reservoir how do you describe the Green's functions that you remember I described the particle and whole Green's function. So, how does that how do those definitions change when the system is in contact with a thermal reservoir exchanging energy in coming to an equilibrium with some temperature t? So, the canonical and symbol idea; so, that I will relegate to the next class.

So, thank you for listening to me, but this particular lecture would have been hard for anyone. And it is not easy to explain this in class. So, you really have to read that chapter very carefully line by line and perhaps even consult some relevant research review articles and only then you will understand the Schrieffer Wolff Transformation. So, but the rest in the next lecture will be slightly easier. So, I hope you will join me for that.

Thank you.