Advanced Condensed Matter Physics
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Lecture – 09
Antiferromagnetism in Hubbard model

So, we have discussed ferromagnetism, now we shall discuss Antiferromagnetism so, what we mean by Antiferromagnetism is that there is a 2 sub lattice in a given crystal lattices, in which one sub lattice call it as, A sub lattice we make this discussion more clear.

A sub lattice contains primarily up spin density or predominantly up spin density and the other sub lattice call it B sub lattice contains pre dominantly down spin density which means down spins. So, you have ordering so, this ordering is up, down, up, down as you go from one lattice site to another and this is called as the Antiferromagnetism

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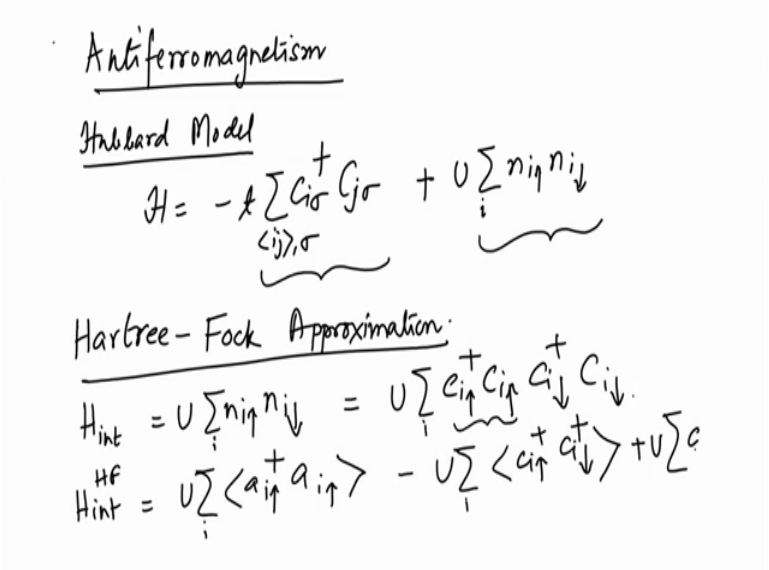

So, we will discuss Antiferromagnetism and again we shall talk about Hubbard model which is what we have done earlier and the Hubbard model is once again for convenience I am writing it as the kinetic energy term which is the first term this term which is neighboring sites hopping between neighboring sites i and j and sigma is a spin.

So, this angular bracket over i j that you are seeing here a, denotes that they are neighboring sites. So, hopping is over the neighboring sites and then we have an interaction which goes as n i up and n i down and runs over all sites i. So, this is the interaction between the densities at a given site. So, this is an onsite interaction between taking place between up spin density and down spin density we cannot have a up spin up spin at a given site which is excluded by the Pauli's exclusion principle

So, similarly now the problem with the solving this model is that you have this term as a 2 particle term which we know that kinetic energy is operators is actually a 2 body operator or rather one particle operator in that sense. So, it causes hopping from one site to another where as if you open this term it will be a 4 body operator and written together you cannot find a suitable basis so, as to solve them exactly.

So, we will not talk about exact solution, but rather what we should talk about is mean field approximate solution and this mean field solution that we are going to talk about now is called as the Hartree - Fock Approximation. So, let us see what Hartree - Fock approximation means now this will be again discussed at length when we do the brains function problem so, Hartree - Fock approximation.

So, by this what we mean is will write down the interaction term or call it H int and so, this is as it is written above it is n i up and n i down and we have discussed this several times that electron density operators can be written in terms of the single particle electron operators as c i up draggers c i up and c i down draggers c i down. So, by this approximation what we are going to do is that we are going to spilt this 4 operator term into 2 operator terms and take all possible combinations that come our way and so, this H int Hartree - Fock is equal to U is the sum over i there is a sum over i and I will take this a i up dragger a i up and plus.

So, the first the combinations are taken with these 2 and then the combinations will be taken between the first and the third. So, I will have a term such as c i up dragger c i down and then there will be a combination taken between. So, this will be this should come in with the negative sign because you have changed to one electron operator you have swapped the c i down with the c i up. So, this should come with the negative sign.

And so, this is the negative and then there will be term which is between the first and the fourth which is again sorry this is dragger and then there will be one between the first

and the fourth so, that cause 2 swaps which would eventually get me a positive sign. So, that is c i. So, I will write it once again I need bigger space so; I will just let me erase this and so, that we can write it slightly elaborately in the next page because I would need larger space here. So, I am cutting it out and let us just go to the next page and write down this.

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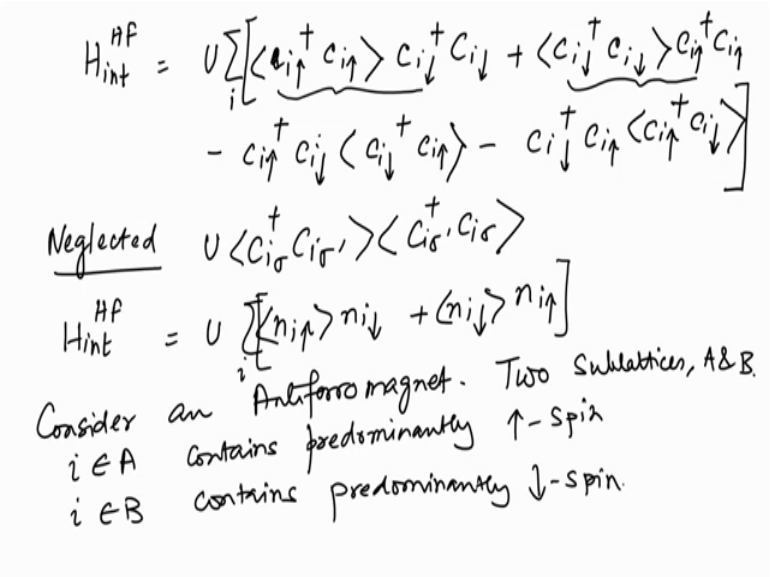

So, H int H F would be U and c i up c i up and a c i down dragger c i down plus c i down draggers c i down and a c i up draggers c i up, now there will be a minus sign because. So, there is a c i up dragger c i down and this comes with the c i down dragger c i down draggers c i up and. So, this and a, another term which is minus c i down draggers c i up c i up dragger c i down.

Now, you see by doing this by doing this we have converted. So, what we have done is that we have taken expectation values of 2 of the operators at a time. So, that the Hartree Fock Hamiltonian can be reduced to a uniformly 2 body term or just like the kinetic energy so, that we can found out a basis and can diagonalise them. So, the 4 operator term has been decoupled into taking a expectation value of 2 of the operators at a time and we have taken all possible combinations in doing.

So, now, it so, happens that the terms which are the first 2 terms that is this terms are important for considering antiferromagnetism where as this other terms are not important for antiferromagnetism, but they are important for something else which we will see

later. So, if you drop these 2 terms and off course there is another term that we are dropping is that when we have the expectation of all the 4 that is 2 at a time. So, there will be a term which is so, neglected term is which is like terms such as this. So, c i sigma draggers c i sigma or sigma prime and there is a c i sigma prime dragger c i sigma.

So, the expectation of so, these are constant terms because we are taking the average values of each of these 2 and it just turns out to be a constant and which is dropped from the problem. But; however, so this total or rather this Hartree - Fock or the interaction term is written as U into n i up n i down and plus n i down n i up and this is our Hamiltonian that we are going to look at along with the kinetic energy term. So, now, consider a specific case as an Antiferromagnet.

So, consider an Antiferromagnet and what we mean by Antiferromagnet is that as I said earlier that there are 2 sub lattices A and B and so, when site is that of A sub lattice then it contains predominantly up spin and a site B it contains predominantly down spin.

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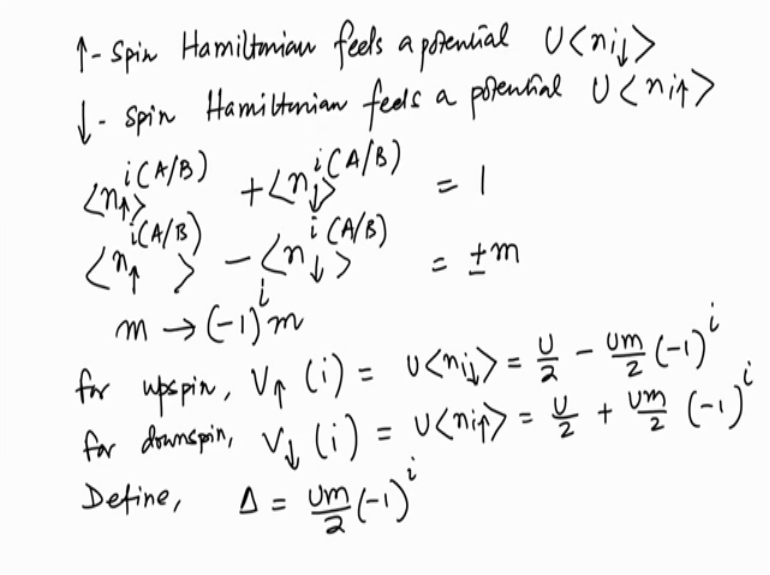

So, if that is the case then we have so, an up spin Hamiltonian feels a potential U into down spin average down spin densities and similarly a down spin Hamiltonian feels a potential U into up spin densities. So, if we introduce notations such as the total density being. So, n up and it is i belonging to either A or B plus n down for i belonging to either A or B should be equal to 1. So, the total density of up spin and sown spin should be equal to 1 as we said that A contains predominantly up spin density.

So, if the site is i site belongs to that of A n up would be much larger than n down and vice versa if i belongs to a site in B then n down will be much bigger than n up, but; however, both of them put together should give me 1 and we can also introduce magnetisation which is given as the difference in these 2 densities so, A B minus n down i A B is equal to m.

Now, this could be the way is written it could be plus m or minus m depending on whether we are on are on the A sub lattice or B sub lattice if we are on the A sub lattice then the up spin density will be bigger than the down spin density and in which case m will be positive and otherwise will have a negative sign here. So, you can see that this whole scenario can be slightly simplified if we write the m as a minus 1 whole to the power i into m; that means, that if we start scanning the lattice site as 1, 2, 3, 4 etcetera will alternately get a b a b a b and so, on.

So, depending on whether we have m i equal to even then will have m equal to positive and if we have i equal to odd then will have m equal to negative so, this is the situation. So, let me go back once again and just let you know that what is my system so, we are planning to study antiferromagnetism and we have written down Hubbard model and we want to understand antiferromagnetism from the Hubbard model just like we have understand understood ferromagnetism from the Hubbard model.

Now as I said that this Hamiltonian cannot be solved exactly because the 1 contains 2 electron operators the other contains the second term contains 4 electron operators. So, it is there is no suitable basis you can solve it one can off course do an exact diagonalisation of the problem which is often done, but it is usually for a smaller number of sites and we want to do it analytically here.

So, we employ a Hartree - Fock approximation which is equivalent to splitting this 4 operator term into 2 operator terms and if we take unrestricted combinations we get 4 terms as it shown here let us call this as equation 1 or maybe we can call this one as equation 1 and this one as equation 2.

So, in equation 2 we have taken all possible combinations and we have said that the only the first 2 combinations are relevant for studying antiferromagnetism and the other 2 combinations are not relevant immediately because they are they correspond to how an up spin is correlated with the an up spin creation operator is created with the down spin

annihilation operator and vice versa and these are not relevant for studying antiferromagnetism because here we are interested in the to see that how a down spin, what a down spin potential is and what an up spin potential is so, that we can write down a Hamiltonian separately for an up spin or a down spin.

So, this is the form of the Hartree Fock Hamiltonian and let us make an assumption to begin with that there are 2 lattice sides A and B and the whole system is formed of interlacing these 2 sub lattices A and B sub lattices. A contains predominantly up spin there could be a small down spin density, but very small and B contains predominantly down spin density and it could also have a small up spin density. So, now, to make notations clear we have written down the total density for i to be in A or B sub lattice equal to 1 and the magnetisation is defined as this.

Now, we have to solve this Hamiltonian because now we have been able to write it in terms of 2 particles 2 operators 2 fermi on operators for each one of the terms that appear there. So, for up spin V up i equal to U into down spin density as we have written which is equal to now from this I solved for each one of the densities. So, these are really the average values that appear there. So, these are averages and this is equal to U by 2 minus U m by 2 into minus 1 whole to the power i by solving these 2 for each one of the n up and n down and for down spin my potential for a given site is U into the up spin density which is equal to U by 2 plus U m by 2 into minus 1 to the power i.

So, these are the potentials for the up spin and the down spin and we have also written it down in terms of m etcetera. Now we can also define a quantity called as the delta so, define delta which will say eventually that it is the magnitude of the gap for an Antiferromagnetic insulator it is U m by 2 into minus 1 whole to the power i that is the second term that appears above and let us keep numbering them. So, let us call this as number 3 and number 4 so, in equation 4 the second term would be replaced by delta.

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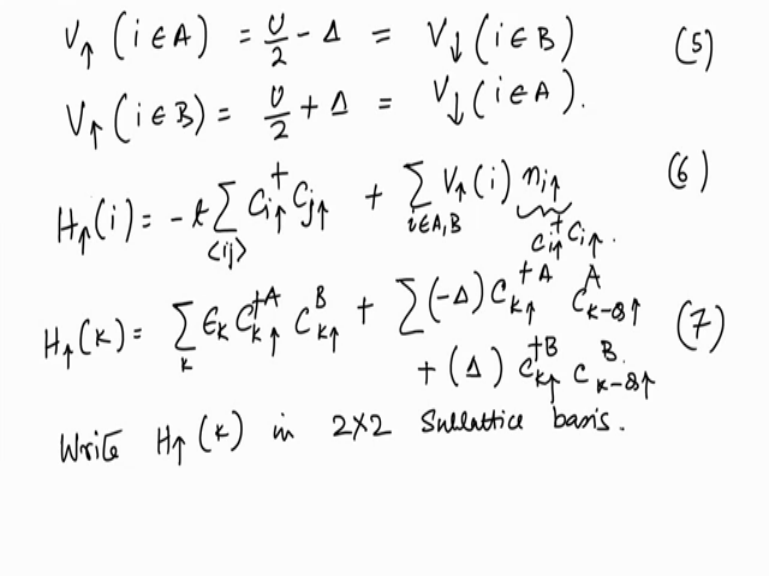

So, that again V up for i belonging to A sub lattice is equal to U by 2 minus delta and this is same as V down for i belonging to B sub lattice. So, there is A sub lattice symmetry which you can see it from here. So, the up spin potential for i to be part of or i to be in their sub lattice is U to U by 2 minus delta which is same as the down spin potential for i to be in the B sub lattice.

And similarly V up for i to be in B sub lattice is equal to U by 2 plus delta which is same as V down for i to be in the A sub lattice and suppose we write this now we can write down the Hamiltonian for each species of spin that is say for up spin. So, let us write down a up spin Hamiltonian to be simply H up i which is equal to a minus t i j now since we are writing it only for up spin we should not write sum over sigma, but it is c i up draggers c j up plus V up and i and it is n i up and this is nothing, but c i up draggers c i up.

So, this is the Hamiltonian for the up spin for i to be any lattice site i can belong to either A or B and if i belongs to A then surely j will belong to B and the visa versa it is true that is if i belongs to B then j will belong to A. Now this way we can also write down the Hamiltonian for the down spin exactly in the similar manner when we will have a simply a all these ups will be replaced by downs and we now know what V up and V down are from the definition that we have given in equation 5 let us call this is equation 6.

Now in order to solve it because we have a 2 sub lattices we can write as a this Hamiltonian as a 2 by 2 Hamiltonian in the sub lattice basis and for that we will have to transform into the momentum space and the momentum space Hamiltonian H up of K is written as K epsilon K C K up belonging to A C K up dragger and C K up in belonging to B and will have up plus and a minus delta term this is for C K up belonging to a C K minus Q up belonging to A and will also have a term which is delta and a C K up belonging to B dragger and C K minus Q up belonging to B so, this is the up spin Hamiltonian.

Now, the sub lattice indexes are made explicit in the super script and there is a off course also a constant term which you will be able to find and will write it the, but the constant term as said is dropped and is not considered in our problem because that will just shift the energy up by a constant term and down by a constant term on little simply a shift. So, it is not important so, what is important is that, we should now be able to write down a 2 by 2 Hamiltonian from the Hamiltonian that appears in 7 and it is it so, write it the task is that write H up K in sub lattice basis and so this H up K is nothing, but minus delta epsilon K let me take out a bit more space here.

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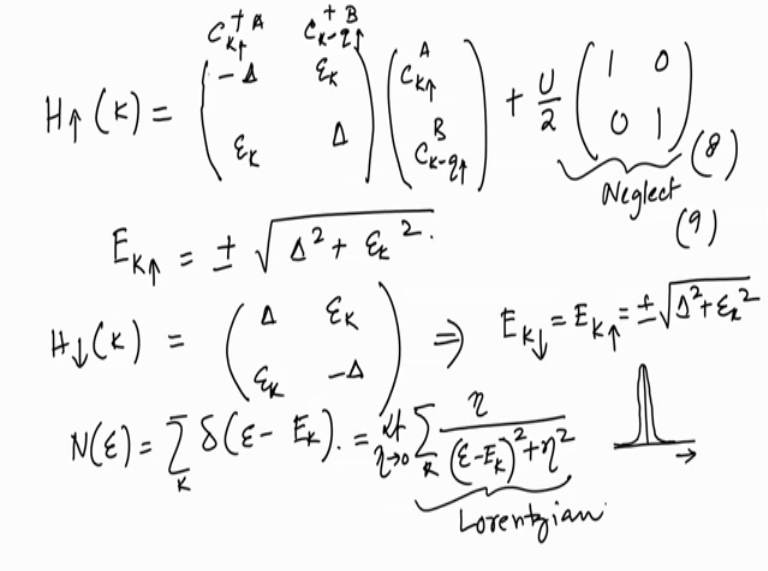

And so, that I can write down the basis also which will help you. So, this is minus delta epsilon K epsilon K and delta and now you will have a C K it is written in C K up dragger A and C K plus q up dragger B. So, it is in that so, it is C K up A and C K plus q

up B and sorry this is not plus this is minus we have written that is minus. So, this is minus and minus here will. So, there is a minus sign here and there is a minus sign here and off course there is a term which we have neglected and we have said that we are neglecting it is term which is like this and this is say equation 8.

So, now, we can so, it is 2 by 2 Hamiltonian and it can easily be solved let me write down the Hamiltonian here this can be solved with the energy Eigen value. So, I am neglecting this part because it is a constant and so, E K if you solve this with this you know how to solve 2 by 2 matrices and find the Eigen values. So, E K up becomes equal to plus minus root over delta square plus epsilon K square and similarly E over H down. So, this is my equation number 9.

So, H down K without the constant term can be written as delta epsilon K epsilon K and minus delta and will again have the Eigen values as E K down which is same as E K up and this is equal to plus minus root over delta square plus epsilon K square. So, this is your solution of the problem. So, do say we have been able to do a Hartee fock decomposition of the Hubbard Hamiltonian and have been able to write it as a 2 by 2 in sub lattice basis and 2 by 2 matrices in sub lattice basis and then diagonalise it to find that there is a symmetry of the up and down spins both give me Eigen values which are same as plus minus delta square plus epsilon K square.

Now, this tells me that this gives rise to density of states how do we calculate density of the states density of states is calculated as N of epsilon which is equal to delta of epsilon minus say E K and this is if you like that this is can be written as there is sum over K and it has to be divided by the for the normalization the number of K points and. So, this is like sum over K and limit eta going to 0 and something like eta divided by epsilon minus E K whole square plus eta square.

This is usually done when you have to calculate the density of states which is an delta function and the delta function will give me a peak as soon as mug the energy will hit a particular value of ep E K and E K will have range of spectrum of values over the full brillouin zone and if you are be a talking about square lattice we have a brillouin zone from minus pi over a to plus pi over A.

Where A is the lattice constant and in order this in order to calculate it computationally a delta function can be delta function is ideally just the straight line having a peak and

infinite peak at particular value of this x axis here whenever omega will hit a key I will get a peak and infinite peaks you have to say and I will have to sum over all these keys in order to calculate the total densities of sates. So, it can be computationally calculated if a give it small width to this by expressing it as a Lorentzian. So, this is the lorentzian and this will help us to calculate the density of states.

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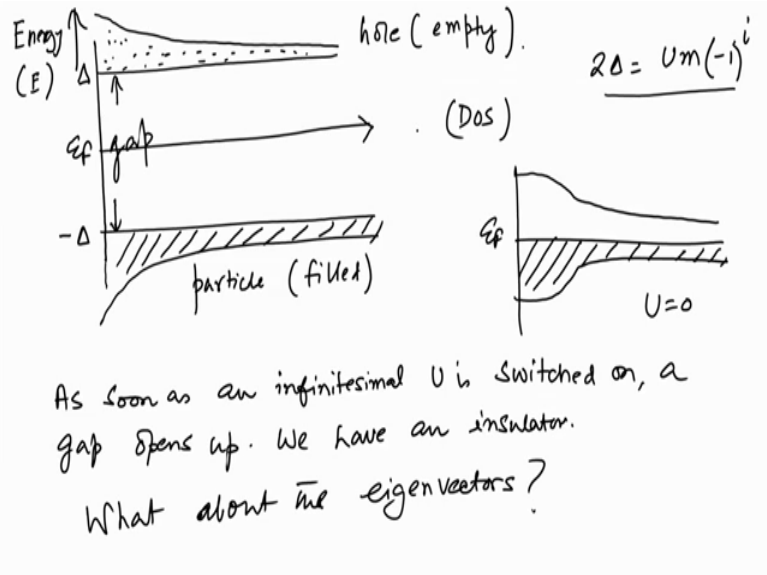

And this density of states comes out as a so, this it will look like this and so, this is the occupied band which is the below fermi energy. So, this is the fermi energy and this is the basically we are plotting density of states verses energy, energy E and this is plus delta and this is minus delta and we have empty whole band which is here. So, this is empty and this is filled so, this is the, it is called as the particle band.

So, it is filled and this is called as the whole band and that is empty ok. So, this is the density of states and this is where the fermi energy lies. So, while write it here the fermi energy instead of there that is the density of states verses energy plot and sometimes you will find that this is the axises turned that is in the x axis energy and the y axis will have density of states, but it means the same thing.

Now you see that remember that we have 2 delta equal to U into m minus 1 to the power i. So, if u goes to 0 that is if you switch off the interaction term in the Hubbard model then you will have only kinetic energy. So, which means that this will this gap will go to 0 the gap that appears here so, this is the gap. So, this gap will go to 0 and will have a

system which is which looks like this which is a metal and so, this is my E f and this is for U equal to 0. So, these are all occupied and it corresponds to metallic vision because you have only the whole states are empty, but there are infinite similar to the particle states so, there are transitions possible between the particle states and the whole states.

The interesting thing is that as soon as and infinitesimal U is switched on. So, I will write this because this important as soon as an infinitesimal U is switched on a gap opens up and we have an insulator, but remember we have started with an antiferromagnetic system.

So, the antiferromagnetism has to show up now going back to this formula we can now drop the minus 1 whole to the power i and only consider the magnitude because we know that it will vary from one site to another it will alternatively become up and downs spin depending upon whether your on A sub lattice or B sub lattice. Now in this problem you have been able to diagonalise it and found out the Eigen values, but what about the Eigen vectors and what do they give us.

So, let us try to find the Eigen vectors.

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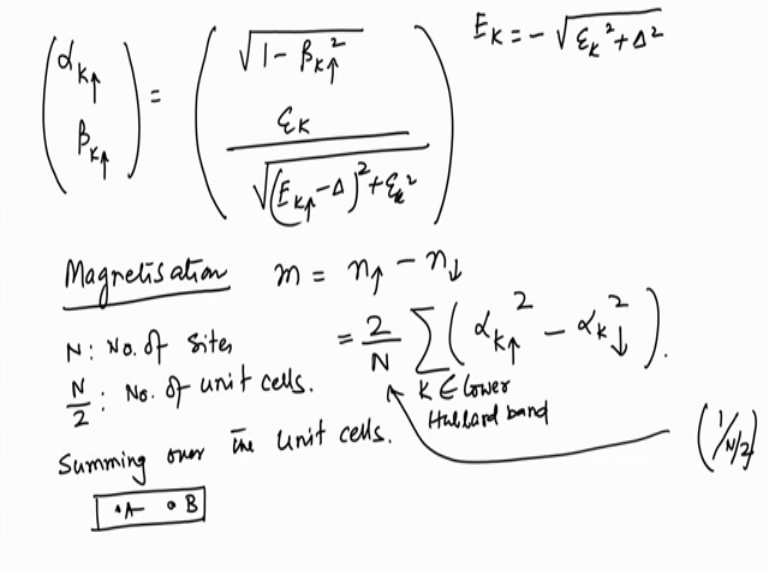

So, let us calculate the Eigen vectors and do a lit bit of a algebra to find out the Eigen vector let us call them as alpha K and beta K for the up spin similarly there will be there for the down spin is as well. So, this we only can calculate one of them because the other

one will obey the orthonormality condition which says that alpha K up square plus beta K up square equal to 1. So, suppose we calculate only beta K and say that alpha K is simply equal to this and beta K comes out to be this you have to do it you have to put one of the Eigen value say plus eigen value and then do it and then also do it for the minus Eigen values. So, we are showing it for the Eigen negative Eigen value which is equal to epsilon K square plus delta square you can also do it for the positive Eigen value things will not be anything different.

So, I have a epsilon K up minus a delta whole square plus epsilon K square. So, this is my amplitude and off course the state will be some amplitude into some space part and in is. So, that could be function of r in some trivial or some non trivial manner so, this is your and then you can calculate the magnetization. So, magnetization is m which is equal to n up minus n down you know that we are talking about a particular site. Now here we are talking about a up spin or a sub lattice site and this will be nothing, but equal to 2 over N, I will tell you why it is 2 over N and K.

Now I will have to sum over all K, but which K is the K is hat belong to the filled band that is the lower let us call it lower Hubbard band or lower band would be sign and this is equal to alpha K up square minus alpha K down square, why it is 2 over N, which means it is 1 by N by 2 the reason is that N is the number of sites and N by 2 is the number of unit cells and so, we are actually summing over the unit cells is that clear so far.

So, we are talking about the magnetization which is the up spin density minus a down spin density and how do we find those densities will have to sum over all occupied levels and we are summing over only the levels which are occupied that is the whole levels are empty and we have N sites off course in the lattice, but there are N by 2 unit cells because each unit cell contains 2 sites each one of A and B.

So, a unit cell contains A sub lattice and the B sub lattice so, this is the A and this is the B sub lattice. So, these are the unit cells for the problem and that is why we are summing over the unit cells and that is why there is a 1 divided by N by 2. So, this N by 2 came from a 1 divided by N by 2. So, this factor has gone in here. So, then we can solve for this and what we can get or what we shall get is the following.

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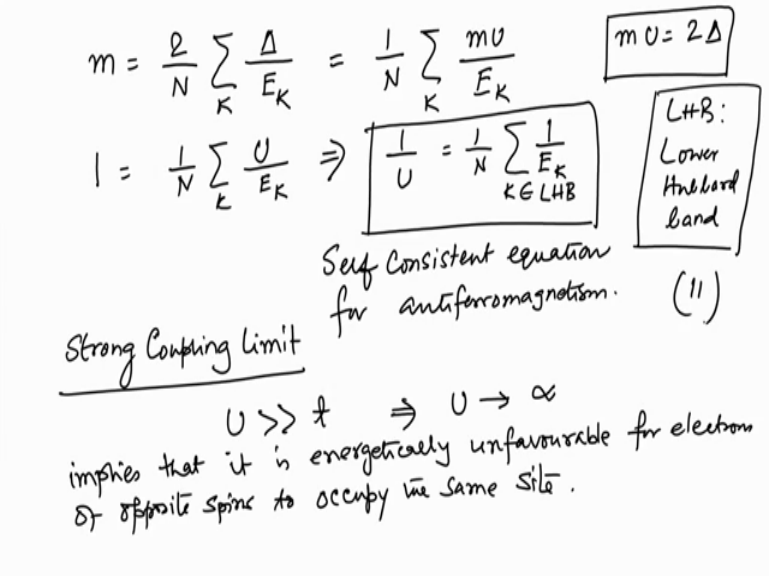

So, will get m as 2 over N and you should work it out to get this as delta over E K so, we are taking difference between the up spin densities alpha K up square minus alpha K down square at a give site which is predominantly containing an up spin ok. So, alpha K down square in principle very small and alpha K up square is large.

So, that I should get a magnetization which is close to 1 and let us see that what happens when we have so, this is nothing, but equal to 1 by N and sum over K and m U over E K because my m U equal to 2 delta. This we have defined it earlier and a since m is not equal to 0, I can cancel m form both sides and I will get 1 equal to 1 by N U over E K or this is recasted in the form that 1 over E K is 1 over N K. Now K belonging to the lower Hubbard band I will write it here l H B means a lower Hubbard band which is occupied.

So, this is equal to 1 over E k. So, just like the stoner criteria we got a self consistent criterion for antiferromagnetism which is similar to the stoner criterion that we have obtained in the last discussion. So, that is myself consistent equation and I should this is the condition for antiferromagnetism to occur.

Now let us see a specific case which is of importance let us call c the strong coupling limit and by strong coupling limit what I mean is that U is much much greater than t and in principle one can just simply say that U tends to infinity. So, the fermi on, the electrons are extremely correlated at a given site.

So, it becomes energetically impossible for if there is an up spin at a given site down spin to come and sit at the same site is nearly impossible. So, this means that implies that it is energetically unfavorable for electrons of opposite spins to occupy the same site. So, if this is the case this is called as the strong coupling limit and or rather strong correlation limit in which case what we have is the following that.

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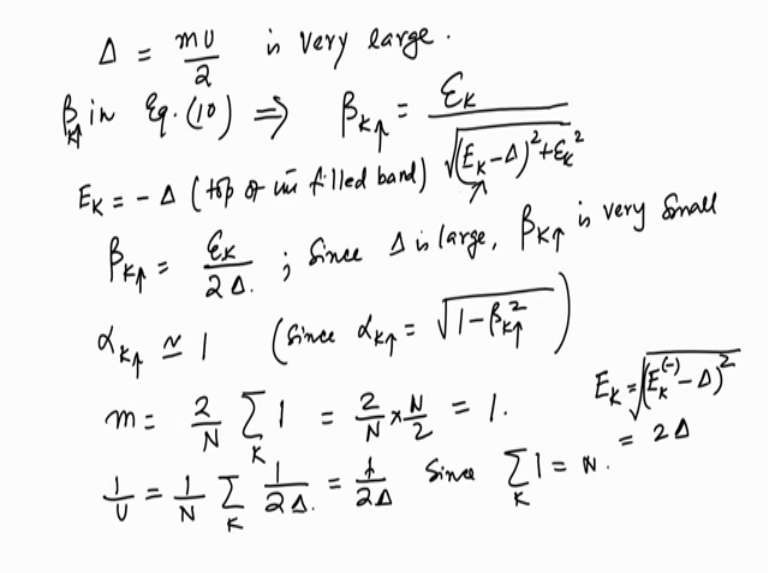

We have a delta which is equal to m U over 2 is very large because U is large and which case let us look at the beta K that appears there. So, we have equation 9 there and let us call this is equation 10 so, the equation. So, beta in equation 10 let us call this is equation 11. So, beta in equation 10 or beta up or beta K up beta K up in equation 10 takes the form.

So, beta K up is equal to epsilon K divided by root over of E K minus delta whole square plus epsilon K square. Now for E K to be which want to consider so, if we take E K to be minus delta, you see here is E K equal to minus delta. So, we take the top of the filled band so, top of the filled band then I have if I put it here then I get a minus delta minus delta whole square which gives me 2 delta whole square which is 4 delta square and that can certainly be much greater than epsilon K square.

So, epsilon K square can be neglected in the denominator. So, I will get a beta K up to be equal to epsilon K divided by 2 delta and this is since delta is large beta K up is very small and this is what we expect that A sub lattice being sub lattice which contains

predominantly up spin the beta K up will be very small and then what we have is that alpha K up in that case will almost be equal to 1 because alpha K is since alpha K up is root over of 1 minus beta K up square and this is nearly equal to 0. So, alpha K up is equal to 1 and if that is the case then my m becomes equal to 2 over N and sum over K now you see that it had this had m U over E K.

So, I can write that as simply as E K to be this can be written as this sum and 1. So, this is equal to 2 by N into N by 2 because sum over K, K over all unit cells and you are summing over 1 which means your summing over the number of unit cells which should give me 1.

So, this is my magnetization so, magnetization is equal to 1 which means that N up minus N down equal to 1 which means N down equal to 0 and N up equal to 1 and the self consistency condition becomes equal to 1 by 1 by U equal to 1 by N sum over K and 1 over 2 delta, now you see that E K becomes E K is same as E K minus delta and that is equal to. So, square root and so, on this is equal to 2 delta. So, this is the self consistency equation and this is nothing, but equal to 2 1 over 2 delta because of since you have sum over K summed over 1 gives me equal to N.

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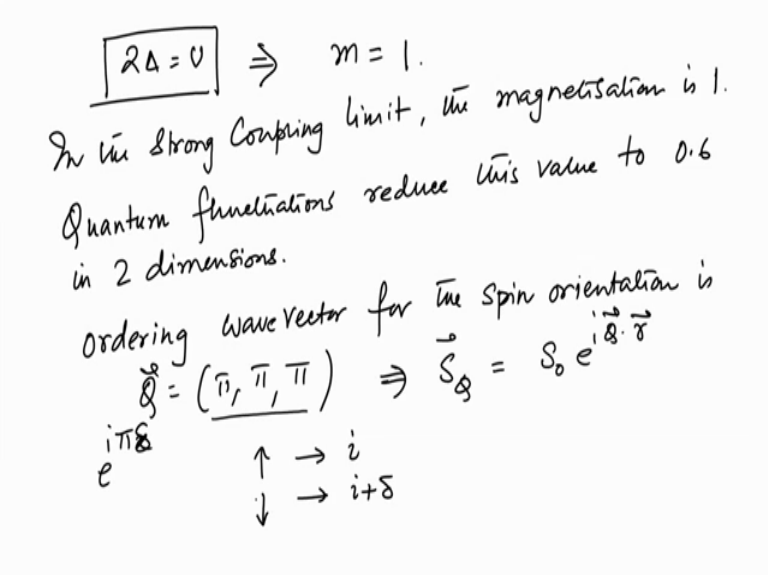

And this is the self consistency condition is that the 2 delta becomes equal to U and that immediately says that m equal to 1. So, in the strong coupling limit the magnetization is 1 this is the magnetization per sites the weights defined as a n i up minus n i down, but;

however, Hartree - Fock picture is somewhat away or some what sort of the realistic picture would be some quantum fluctuations associated with it, because it is a mean field picture or a average field picture and this because of the quantum fluctuations is value of the magnetization goes down and these quantum fluctuations we are not including it, but we will learn later how to include quantum fluctuations.

So, quantum fluctuations reduce this value to a 0.6 in 2 dimensions. So, in 2 dimensions the fluctuations are large so, this quantum fluctuations actually reduce the value by 40 percent and the magnetization will be in the strong coupling limit the magnetization will be 0.6 that is the sub lattice magnetization.

So, this gives rise to an ant ferromagnetic insulator as soon as you switch on a U it will be an insulator and each site will order the A sub lattice will have a up spin density B will have down spin. A will have up spin again and B will have down spin and this corresponds to ordering vector which is given by.

So, ordering wave vector wave vector for the spin orientation is S Q equal to pi, pi, pi let us just try to see it in one dimension how it looks like. So, in one dimension will have sort of so, this enables us to write S Q equal to some S and 0 and exponential i Q dot r. So, this is how the profile will go and so, in one dimension if I take a exponential i pi x as the modulation, this i pi will give me negative sign.

So, as I go from one site to another I mean I have to write this as delta so, this will be a delta. So, how the, if I have an up spin at a given site i, i plus delta I have a down spin right. So, the ordering becomes so, as I go from up i to i plus delta i should get from the ordering of the spin.

The spin vector will change it is orientation from up to down and that is why this pi, pi, pi that kind of a ordering will come and this can be actually probed in from scattering experiment. So, the neutrons scattering experiment will detect these Eigen vector and see that there is a ordering of this kind in the 2 dimensional plane it is. So, in order to do neutrons scattering for a 2 dimensional thing one has to actually take a small angle neutrons scattering so, that you can see the surface well so, the spin orientation in the surface.