Electronic Theory of Solids
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Lecture – 45
Ferromagnetic Heisenberg Model

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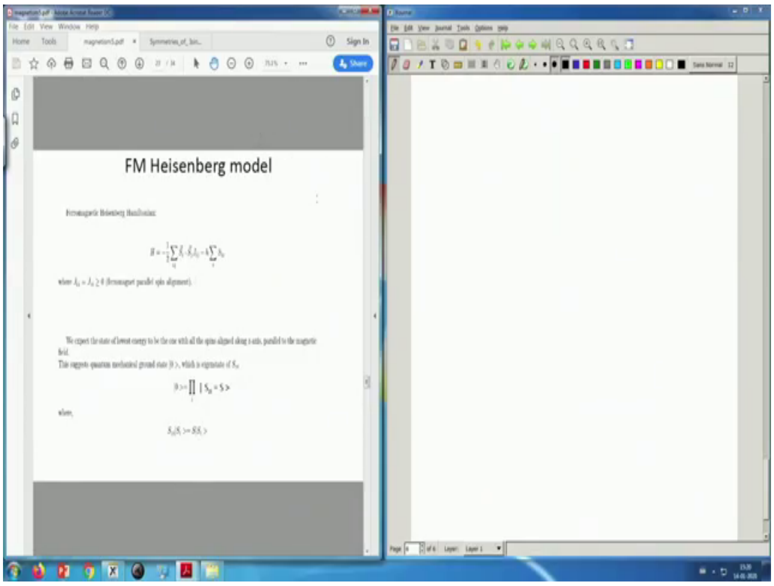

We have been discussing Ferromagnetism starting from Heisenberg model. So, our purpose is to try to solve Heisenberg model if that is possible and I argue that it is not difficult to solve the Hubbard model in the ferromagnetic limit. While it is extremely difficult to solve Hubbard model in the anti ferromagnetic limit and indeed anti-ferromagnetic Hubbard model sorry anti-ferromagnetic Heisenberg model has been solved only in one dimension by a very famous calculation which is done by Hans Bethe in 1931.

And that method is an iconic method in the mathematical physics of this kind of models and that is called Bethe ansatz. He used an ansatz to solve this problem. It stood the force mathematical calculation and it is a hallmark of a genius doing mathematical physics and he is of course, a one of the great physicists of the last century.

The point is that the Heisenberg model in the ferromagnetic limit which means all J ij s are positive is not so difficult to solve and then we try to solve it using our intuitive understanding of what should happen in this kind of a model. Remember classically you can easily guess what is going to be the solution. It is interesting that for ferromagnetic Heisenberg model your classical guess works out and that is this that is the quantum ground state as well as we will so show below.

Now, how do we choose this ground state ok? So, we have to choose a quantum mechanical state and wave function for the entire spin system which is basically thermodynamic in number. So, you choose this ground state based on your classical assumption that you see if all the GIJs are positive, then this Hamiltonian should give me all spins up and that should be the lowest energy state and magnetic field of course, chooses what is the up direction.

So, that is the direction we call up z direction ok. Now how do I write such a ground state. Well that is not difficult we what we do is that you just come to every site, take the projection of the spin along that z direction and make it maximum as large as possible and what is that maximum value that value has to be S the value of the spin. That is a maximum projection that you can have.

So, S is actually S is given by the maximum projection and so that is the maximum moment that you have at each site in the direction of the field and so you just take that and take a direct product of all these states in the to form the ground state ok. And to be more precise because it is we are doing quantum mechanics, I also define the operation by the operator S z of the ith site at the at this state at is at the S z i equal to S at the ith site and that state that operation will give me just the maximum value of S which is S.

So, S z operating on S will give me S if the projection is maximum which is S and that is what is written here ok.

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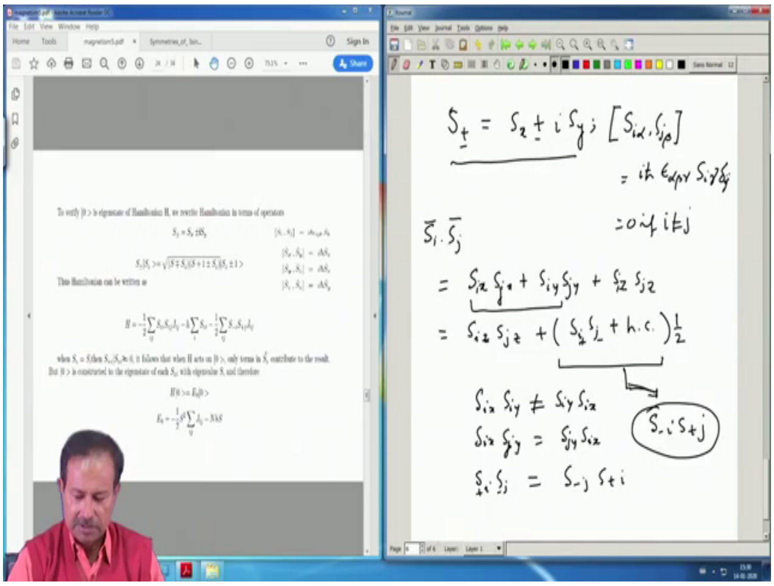

So, that is the starting point. Now we want to rewrite the Hamiltonian. How do I rewrite the Hamiltonian? Well, the standard method is to use these operators raising and lowering operators which you are familiar with in quantum mechanics which are Sx plus minus i Sy at every site.

So, for i'th spin I will do I will just put an index i here ok. So, how does it help? Well, I will just show you how does it help, but before that let me just write down the as I wrote down earlier the commutation relations are like this S i alpha S j beta equal to ih cross epsilon alpha beta gamma S gamma S i gamma ok. Now if i and j are different then of course, I have to put a delta ij here.

So, if i so, that is equal to 0 if i not equal to j ok. So, that is the caveat that one has to remember and that is something I will be using in this derivation of Heisenberg ferromagnet ok. So, let us write down this term S dot S i dot S j as S x ix S i S jx plus S iy S jy plus S zi S jz. So, so that is just the dot product of these two, but then what I will do is that I will keep this of course, intact, but I will write this as a combination of S i plus S j minus plus the Hermitian conjugate of that.

This I will leave you to go through. Remember that there will be a half. So, this will be this you can show easily basically write S as this and this is just the Hermitian conjugate of this operator and then you what all you do is just take the product just do the algebra and what you will find is that this reproduces these two terms ok. So, because it is the other thing that you have to remember that since i and j are different sides, you can always commute these spins.

For example, S ix S iy is not equal to S i y S ix, but S ix S jy is equal to S jy S ix because they commute. So, that is something you can use and; that means, S plus at site is minus at site j these will. Sorry I am using up and down at the top. As denotation I am using is plus here and minus here. Similarly here also I will do the same thing. I will write plus minus here plus minus S plus minus ok.

So, this can be written as S minus j S plus i because they i and j are different sites. So, these things come in. So, if you do that then what you will end up with is a Hamiltonian of this kind. So, you can you can just commute and then what you will have is the idea is that why do you want to write it in this way. The main purpose is to write this term this term as some S minus i S plus j that is what we are trying to do, this term.

You will immediately see when I go to the next step why one wants to write this and this is the term that is do you can write using these commutation relations and you can just switch the terms in such a way that the plus j appears on the right ok.

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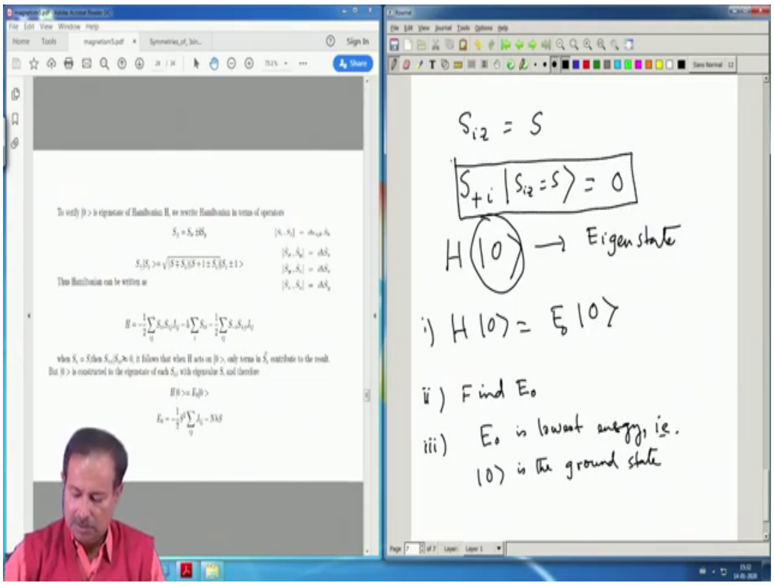

Now, let us go to the next step. When S z suppose at a site i S z is equal to S well at site a then in that case if I apply S i on that S i z equal to S then I will get 0 because this is the maximum value of S already attained by this z component. If I want to raise it further, I will not be able to do it. So, I will get a 0.

So, that is the reason I have taken S plus on the right hand side. So, now, if you look at this Hamiltonian if this Hamiltonian acts on the ground state, then I need to do two things. One I have to first show that it is an Eigen state that it is an Eigen state. This one is an Eigen state. So, to do that I have to show that H 0 equal to sum E times 0. So, this is something I have to show that is number one.

Number two find E 0, and then of course, to show that this is the ground state then I have to show that E 0 is the lowest energy state. So, that is all we are doing. This is in ground state we are trying to figure out what is the ground state. So, there are 3 steps one is that I will this use the Heisenberg Hamiltonian to operate on this chosen state 0 and first I have to show that the chosen state is indeed an Eigen state. Second, I will have to find out the eigen value and third is that I have to show that there are no other states which gives a lower eigen value.

So, the E 0 is the lowest energy state lowest energy. Sorry, E 0 is the lowest energy and that is 0 is the ground state. No other state has lower energy. So, these are the 3 steps we I am going to take now because of this property.

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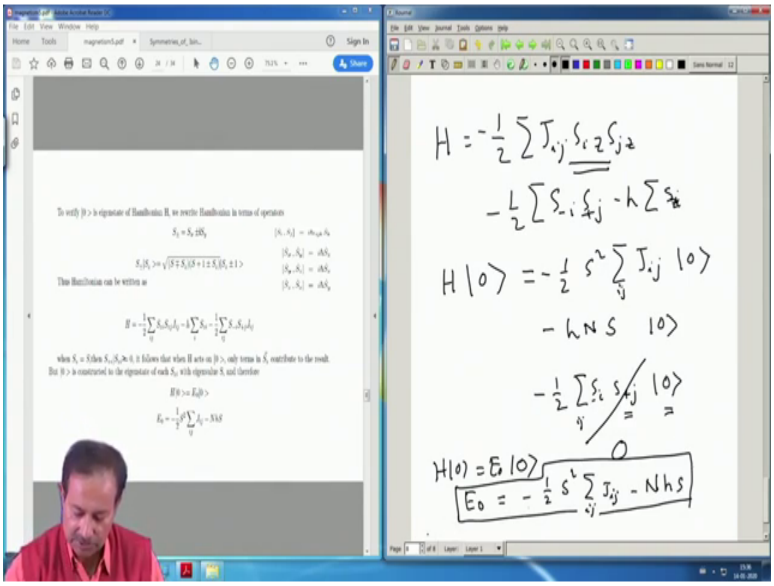

If I apply the Hamiltonian on that state 0 H operating on 0. H has these two terms half J ij S i z S jz minus half S minus i S minus plus j. This operator and minus H times S i z. Sorry S z i, then I will just operate this on this.

Now, let us see what these terms give. See these are both z S z operators. So, that will simply give a square from here right so, minus half S square sum over J ij. So, that is the first term and that will of course, give me max 0. So, that is that part gives me the is like an Eigen value equation. Let us look at the second part the third part which is again S iz. So, that will again give me sum over i basically all S. So, every sum every spin will give me S operating on 0.

So, this will be N times S. So, I can straight away write this as N times S. N is the number of sites ok. So, this is H N times S. Now I have the other term minus half. This term S i minus S j plus ij operating on 0; this term will immediately make all these at every site this will make it 0. So, this contribution is just 0. So that means life is so simple now. Because of this particular construction the way I have read it in the Hamiltonian, it be life becomes so simple. So, now I can see that it is an Eigen state.

So, I so if I write H 0 equal to E 0 then my E 0 E 0 is minus half S square sum over i j J ij minus Nhs. So, that is the. So, the first one 1 and 2 that it is a ground state. So, I have established two things. There is I have not yet established it is ground state I have established that it is an Eigen state. So, 1 and 2 are done that 0 is an Eigen state 2 E 0 is equal to whatever we found out right minus S square J ij minus Nhs.

The third one is still to be shown that this is the lowest Eigen value that you can ever find for this model with ferromagnetic js. So, that is the thing that we have to do now.

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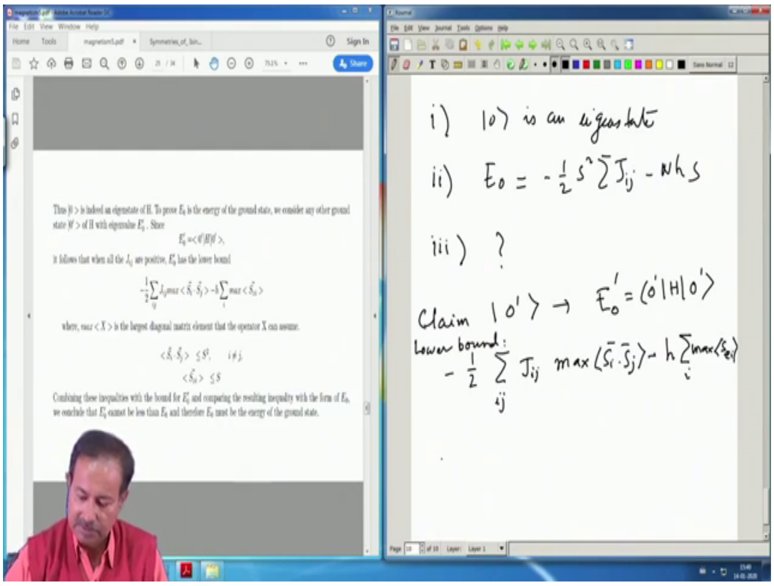

So, to do that one it uses a small trick that is one tries to write down an another state. Suppose I can write down another state and I claim that it is energy is lower than this energy E not.

If I can show that then of course, I I can I will immediately disprove this assertion that this ground state that I have chosen is not the right ground state. There are states which are with energies below this ground state. But suppose I cannot prove that and I can show that this is the lower bound of any state any energy that you can any Eigen value that you find for any other state this is the lowest bound that you can have then of course, I am home I can claim that ok.

So, that means this is the lowest energy Eigen value and therefore, this is the ground state. So basically I will have to show that there is no other state whose energy is lower than this. So, let us just claim. So, I claim there is a state called 0 prime whose energy is lower than so lower than E 0. So, E 0 prime which is equal to 0 prime H 0 prime is that a my claim would be that this is the lower this would be I want to show whether this is lower than E 0 ok.

So, let us just write the Hamiltonian again. If all the J ijs are positive which is what we are doing then of course, this is the lower bound of the energy J ij maximum value of S i dot S j right minus H times maximum value of S i S zi. So, this is obviously the this is the lowest energy you can think of right you can have because maximum value of this with a minus sign maximum value of this with a minus sign.

So, suppose I want to find out and I claim that E 0 prime is a state for which is this which whose energy is this E 0 prime is this energy. So, I will find this is the maximum this is the minimum energy that you can think of and then I will try to see if that minimum energy is bigger or less or equal to E 0 ok. So, that is what I will find out.

So, upper bound,. This is the upper bound. This is the lower bound of the energy right ok. So, what is this maximum of S i dot S j so that requires some calculation. Let us just try to outline how you do it.

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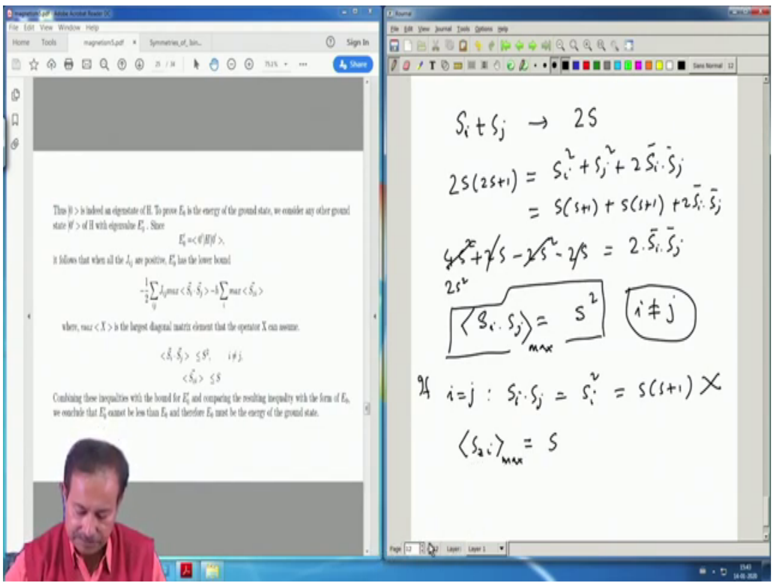

Remember S i plus S j this can form both of them are S. So, the maximum they can have is 2 S ok. So, then S i plus S j square is 2 S into 2 S plus 1.

So, the square of this is 2 S plus 2 y and this is equal to S i square plus S j square plus 2 S i dot S j. So, I have already I have the maximum on this side. Now these two are basically S into S plus 1. So, S into S plus 1 plus S into S plus 1 plus 2 S i dot S j. So, this I bring on to the other side. So, 4 S square plus 2 S minus 2 S square S plus S minus 2 S equal to 2 S i dot S j.

So, that means these give me 2 S square and these 2 cancel. So, S i dot S j equal to S square. So, that is the maximum that you can have S i dot S j fine. So, maximum of S i dot S j is S square. The only thing you should remember that i is not equal to j here. If i were equal to j if i equal to j then we already calculated this we know because we are using it.

So, in that case it will be just the you can easily calculate it right I mean it is i if i equal to j then this i is just 2 S 2 S i. So, S i square is S into S plus S plus 1 ok so, ok. So, this let me just write down again. So, if i equal to j then what do you have then S i dot S j s i dot S j is S square right. Because it is just S i square and that is equal to S into S plus 1.

So, that is if i equal to j, but that is not the situation we have ok. So, what we have is i not equal to j and this is not the situation we have and so this is the maximum value of this operator j max of S i dot S j. And the the maximum value of S z i is how much that is of course, S.

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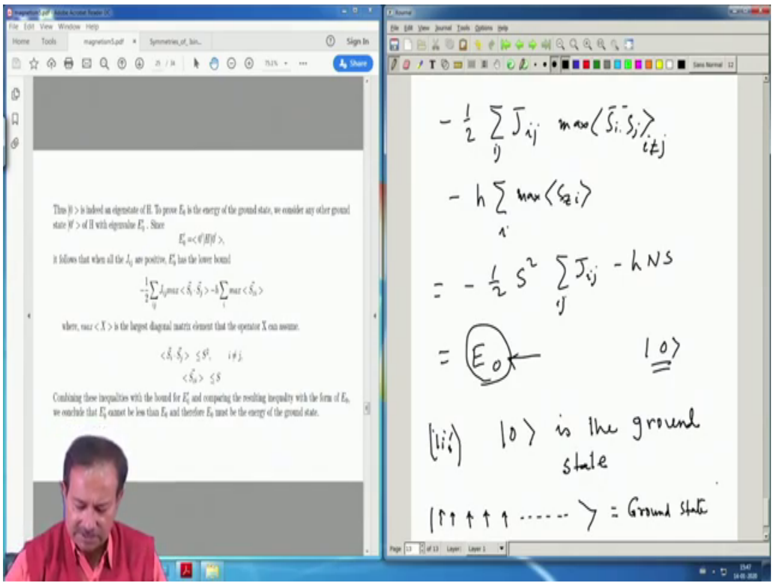

So that means this thing that the minus half J ij maximum of S i dot S j i naught equal to j remember minus h sum over i maximum of S zi is equal to minus half S square J ij sum over ij minus hNs.

Now, look at it this is equal to E 0 that we obtained for our original ground state classical ground state that we that we made an assumption that that is the same state that will apply here. Our chosen ground state which was this this ground state for this is the same energy. So, the the lower bound of the energy of this Hamiltonian a it coincides with this value.

So, the lower bound being equal to E 0 there is no other state there is no other energy or state for which the energy is below this one. So, that means this E is the ground state ok. So, that is how these calculations goes and so number 3 is also now proved. So, number 3 which is the ground this 0 is the ground state. So, that has now been proved.

So, we set out to do calculations on Heisenberg ferromagnet and what we found out is that indeed the chosen ground state where all spins are up with full value of spin S is indeed the ground state. So, this is a very lucky situation where your classical intuitions work out and give you the ground state the right ground state the that E is the ground state where the classical ground state and the quantum ground the by classical grounds time I mean the classically a state which is the lowest energy is all the states all the spins are up. In quantum mechanics of course, I have to write a corresponding wave function and that is this direct product wave function of all the spins being attaining its maximum z component value and the that ground state which is the classical analogue indeed E is the ground state.

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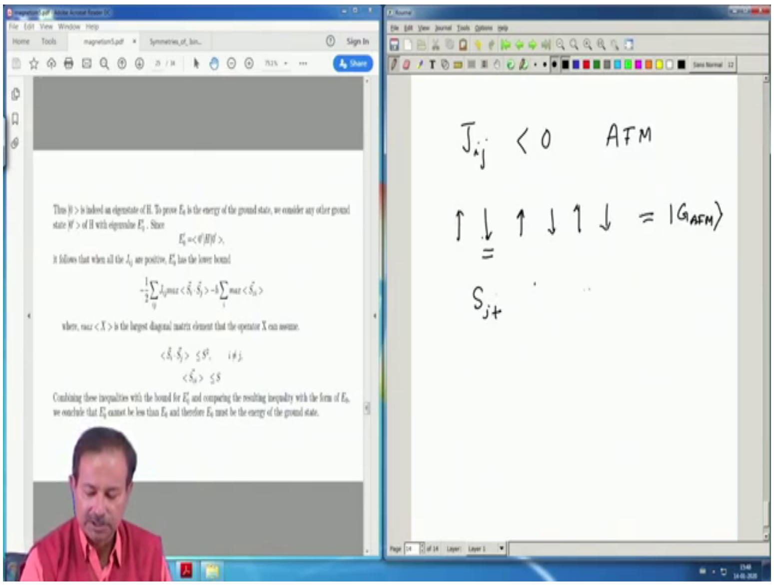

So, for this case we are extremely lucky that we found the right ground state, but suppose these J ijs are negative. Then of course, you have an anti ferromagnetic situation right. Spins alternate spins will be like up and down up and down right. So, in one dimension for example, this is how it should look like classically that is what our intuition tells us. You can of course, write this state as a product state again, but what we will find just do the same thing that I did just operate with h as I wrote down and then you will see that this S j plus operator operating on these spins will not be 0 it will just raise the spins back to it is just reduce the value of S from minus S 2 minus S plus 1.

So, in spin half case this will just reduce from we will go from minus up 2 plus up; that means, it will just turn back up. So, it is not 0 and then if it turns up then of course, you have a different state. So, you are operating on 1 on this ground state you will not get back. So, suppose this is the ground state new ground state for AFM that the ground state for AFM that you chose then the Hamiltonian operating on G AFM is not some energy E times G AFM.

So, it is not even an Eigen state. So, that is a big problem and that is that says that this state is not the not even an Eigen state. So, let us not even bother about whether it is the ground state or not and that complicates life a lot. So, I will not get into that as I said only in one dimension there exist a solution for that state.