Electronic Theory of Solids
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Lecture – 37
Exchange interaction for 2 electrons

Hello and welcome, we have been discussing magnetism so far and we will continue to discuss it for few more hours, one or two hours.

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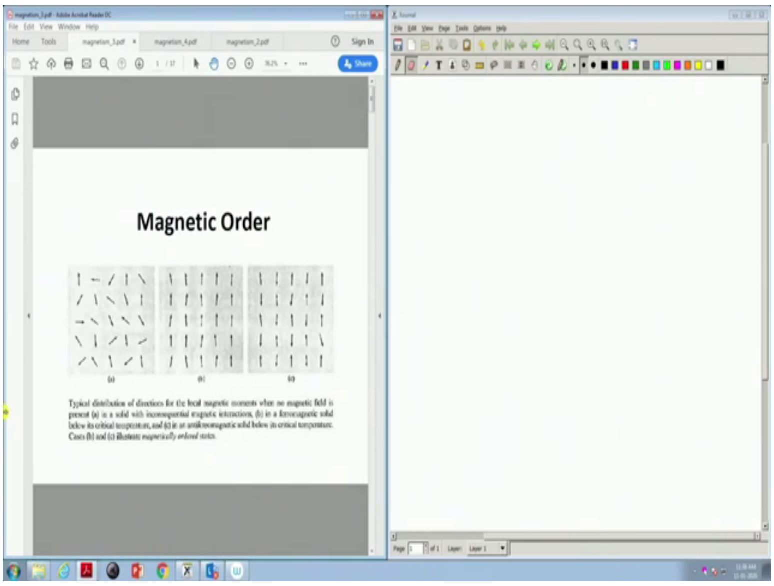

Magnetic Order

Typical distribution of directions for the local magnetic moments when no magnetic field is present (a) in a solid with inconsequential magnetic interactions, (b) in a ferromagnetic solid below its critical temperature, and (c) in an antiferromagnetic solid below its critical temperature. Cases (b) and (c) illustrate *magnetically ordered* states.

And the reason for that is that, magnetism is so vast and it is one of the major areas where both theory, experiment and applications are being developed almost every other day; that this subject needs constant study and one has to at least know the basics of magnetism, particularly magnetic interactions, magnetic order, and how they can be used.

And in this there is a vast literature on magnetism and we are just covering the basic ideas of magnetism therefore. And so, let me start by reminding you what we have done; what we have done so far is simply that, we started out by writing the magnetic Hamiltonian of an electron in an ion or an atom. And then tried to understand the kinds of magnetic response that these ions or atoms with their electrons give rise to. And we found that there are two major kinds of response; one is a paramagnetic response, one is a diamagnetic response.

The paramagnetic response is where the magnetic moments try to align with the field; but the diamagnetic response is where the magnetic moments try to missalign with the field. Or if there is no moment in the atom, then the electron orbits react like as in lenz law against the magnetic field and develop a magnetic response. And that magnetic response is the diamagnetic response, which is opposite to whose corresponding susceptibility is negative while that of paramagnet, where the already existing moments react with the to the magnetic field positively with the positive susceptibility.

So, that is the main difference, apart from the fact that the paramagnetic response is enormously larger compared to the diamagnetic response. Remember the diamagnetic response exists in every case, it is always there; but it is magnitude is exceedingly small if paramagnetic response exists. And so, that is the; that is what we did for isolated moments, which are there in a solid for example.

The next thing we did was to do a calculation for the susceptibility of it is of such a system of moments which are independent of each other, they do not talk to each other, and they are in thermal equilibrium at a particular temperature. So, and if this thermal response is important, because these magnetic energy scales being not very high; the temperature basically has higher energy scale comparable or even more than those energy scales.

And therefore, the randomizing tendencies of the temperature, thermal fluctuations are very important and one has to find out how the competition between the fields propensity to align magnetic moments and temperatures role as a randomizer they compete, how they compete and what is the outcome. And what we found out was that, there is susceptibility then goes as 1 over T and that is a very famous relation first obtained by Pierre Curie and that is called the Curie’s law. We calculated it for s equal to half, moment equal to half, j equal to half for example and for any arbitrary j; and in both cases of course, apart from some numerical factors, the relation still is chi going as 1 over T.

Now, this of course, is it is a celebrated relation, but unfortunately it fails for metals. And the reasons are quite clear that, in a metal the response of the conduction electrons is very different. And they are different because of the same reason that the we found out specific heat for example, was not a temperature independent constant; but it goes linearly with temperature and it is way below the values that we obtained classically. So, that same argument can be brought forward here, and that argument tells us that look there is a in a metal the conduction electrons form a degenerate pharmacy, where all the states below the Fermi level, Fermi energy are occupied. So, the up to Fermi surface all the momentum states are occupied and so there is a Fermi energy.

And this, that means, the excitations are restricted to region to states above the Fermi surface. So, all excitations that take an electron from one state below the Fermi surface to another state below the Fermi surface are not allowed. So, that restricts the phase space enormously and that is exactly what happened in when we calculated specific heat using quantum mechanical systems for quantum mechanical systems, which this a degenerate Fermi surface Fermi sea is.

And similar arguments apply here and then what Pauli showed was that, his own principle which is Pauli principle comes into play as in the previous case, as in specific heat and restricts the phase space. And only a few of the fraction of electrons which is k B T by E F can participate in the magnetic response. And their response is again curie like; but then there is a factor of k B T by E F multiplying that and so, the temperature cancels out and you get a susceptibility which is temperature independent and proportional to the density of states at the Fermi level.

So, this is what we have seen so far; a large magnetic large amount of magnetic theory goes into understanding a another class of system which is the magnetically ordered system; systems which is spontaneously magnetically ordered, you do not need a field to order them. And these are I introduced the in the last class that, these are systems which we are very commonly occurring and they are; for example, iron, nickel, cobalt and their oxides which are added some of them an anti ferromagnetic.

So, iron, nickel, cobalt for example are Ferro magnet, with magnetic order, which is shown here. So, this is the middle curve is the b is magnetically ordered, ferromagnetically ordered c is antiferromagnet and so on. And a is paramagnet, where moments exist; but they are randomly directed, so the net moment is 0; moments exist on a on ions or atoms, but they do not order. Whereas in b and c they do order; were as although in b we will find a net moment, in c would not you would not.

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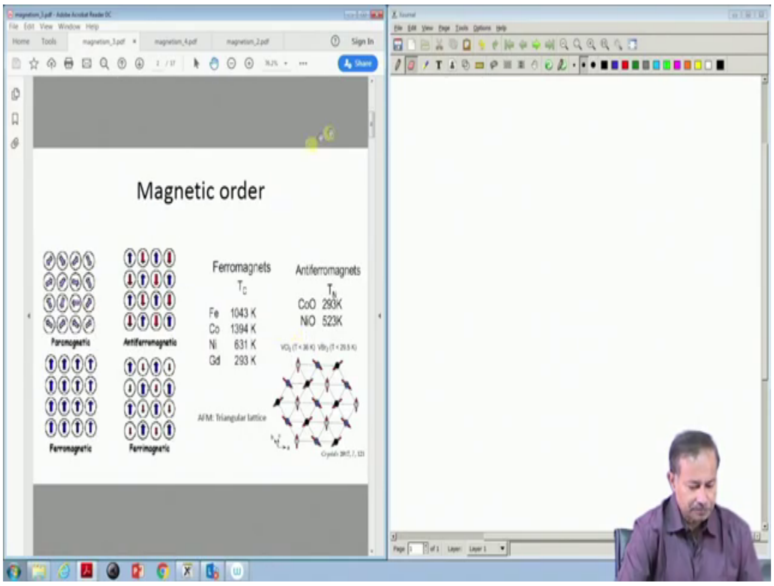

Magnetic order

Ferromagnets

T_C

Fe	1043 K
Co	1394 K
Ni	631 K
Gd	293 K

Antiferromagnets

T_N

CoO	293K
NiO	523K

So, this is a better picture in that sense with colors, this is this again depicts a paramagnet the left top; then there is a ferromagnet bottom left, and this is antiferromagnet where you can see that the this is all done on a square lattice. So, the moments are placed on a square lattice. So, here for example, in this case all the ups pins have their nearest neighbors as down spins; but spin I mean moment typical electrons have spin half.

So, one in that case if spin and moment are interchangeably used, and so nevertheless these are; the moments are aligned opposite to each other and on a square lattice and even on a cubic lattice, you will find that all moments in an antiferromagnet with one direction have their neighbors having moment in the opposite direction.

So, these kind of lattices are called bipartite, they can be partitioned into 2 different lattices. If you look at this blue spins; for example, they also form a square lattice rotated with respect to the original lattice, and the red lattice red spins also form a square lattice, but again rotated. So, there this original lattice is actually a interpenetrating two different lattices. So, it is a sum of two interpenetrating square lattices.

So, in such lattices you can have, every up spin will have it is all neighbors down spin and vice versa. There is this class of materials, where there is there are typically this ferromagnetic structure is where are the up spin and the down spin are exactly like antiferromagnet, but their magnitudes are different.

So, the net moment does not cancel like in antiferromagnet; this happens generally in systems where you have two different kinds of atoms in these two sides; one carrying a moments in J, another carrying a moments J prime which are different and they are antiferromagnetically coupled. There are these examples I gave that, this ferromagnets for example, with Curie temperatures with transition temperature. So, what is transition temperature? The transition temperature is basically a temperature above which the randomizing the tendency of randomization by thermal fluctuation wins, wins over the ordering properties of this material.

So, when something orders there must be a scale right that is that interaction, there is an interaction that tries to order these magnetic moments and that sets a scale; and that scale has to be surpassed by temperature to make the system random. So, for example, in iron below 1043 Kelvin the magnetic moments start ordering; you will find a finite magnetic moment, if you do an experiment on this, on an iron. And above 1043 degree Kelvin, the system becomes a paramagnet; moment still exist, but there are they have become randomly oriented, they fluctuates because of thermal fluctuations and the net moment turns out to be 0.

Similarly, for cobalt it is even higher 1394 degree Kelvin. So, these are these numbers 1043, 1394, 631, 293 all these tell you what is the scale of interaction that tries to, or that is trying to order these spins, ok.

So, see it is a scale of ordering and the disordering tendency of temperature has to overcome that to give you a paramagnetic state. So, this transition temperature is what is referred here. So, this transition temperature actually tells us that, there is a there is an interaction which tries to order whose scale is of that magnitude somewhere close to that magnitude.

For antiferromagnet there are these cobalt oxide, nickel oxide, manganese oxide and so on they are all antiferromagnet and these antiferromagnets look like this for example. So, their ordering temperature is somewhat lower here and the, this again sets scale as to what is the ordering energy. So, the there what is the underlying interaction that is. So, two things one has to find out; what is the underlying interaction that leads to this kind of ordering, and what is its scale and the scale is already given by these numbers. T sub N is the standard notation for antiferromagnets, the transition temperature for antiferromagnets; this is after Louis Neel who did the pioneering work on antiferromagnets.

This is a special example I gave is a triangular lattice where the spins are, see this is not a bipartite lattice. So, in this case you cannot divide the lattice into two independent, as a sum of two triangular lattices; this is one triangular lattice and these are non bipartite lattices. And here the this particular state that is shown is called the 120 degree state and it is an antiferromagnet; but because you will find near no net moment and each spin is rotated from it is neighbor by 120 degree. So, this is this is actually what happens in for example, V Cl 2 or V Br 2 with fairly low transition temperatures. We will come back to these systems later on.

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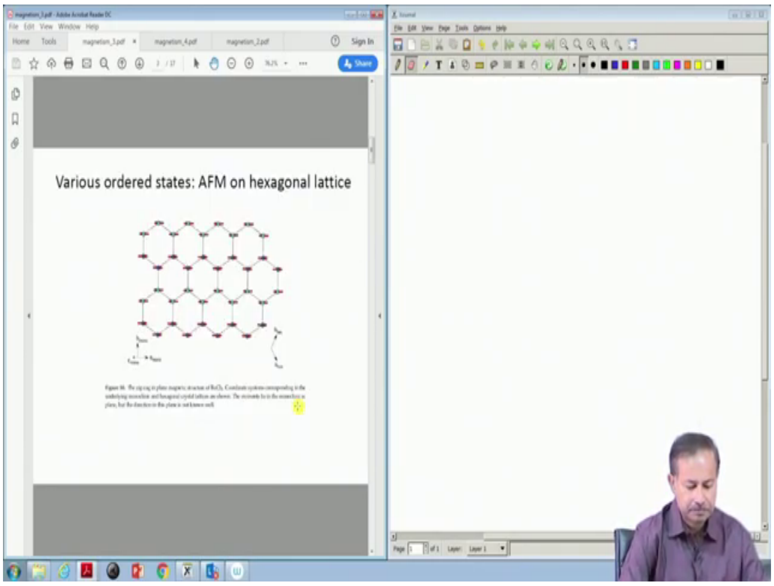

Various ordered states: AFM on hexagonal lattice

This is another example of a of an antiferromagnetic state on a hexagonal lattice and look at this antiferromagnet, it is not that all nearest neighbors of a particular spin are in the in opposite direction; this there is a row which is where all spins are aligned in the same direction, the next row is where the spins are in opposite direction, but they are all aligned.

So, the net moment if you sum of these moments, you will still get 0; because this row will cancel with this row, this next row will cancel with the next row and so on and so forth. So, this is a different kind of anti-ferromagnetic order.

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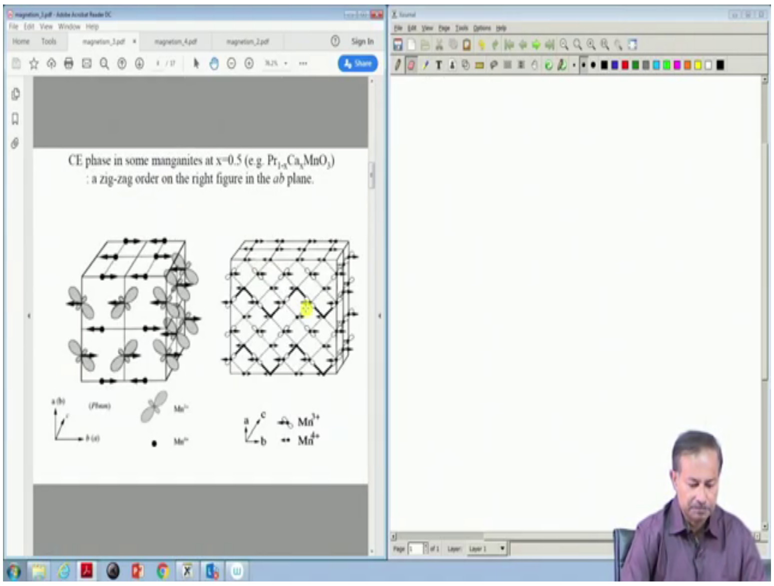

CE phase in some manganites at x=0.5 (e.g. $Pr_{1-x}Ca_xMnO_3$)
: a zig-zag order on the right figure in the *ab* plane.

There are many more , there are very exotic magnetic phases as some of which I listed , I have given here, shown here; these this is so called CE phase and there is a zig-zag order as you can see on the on this face in the so called a b plane in this picture. And these are orbitals that are drawn d or corresponding d orbital’s, where the spin is sitting, we will not discuss it now.

But just look at these arrows, these arrows are pointing in such a way that the total moment is still 0. So, this is an anti ferromagnetic state, but this is called CE phase. It happens, it occurs in systems like manganites at around half filling, so this is an exotic state which is obtained.

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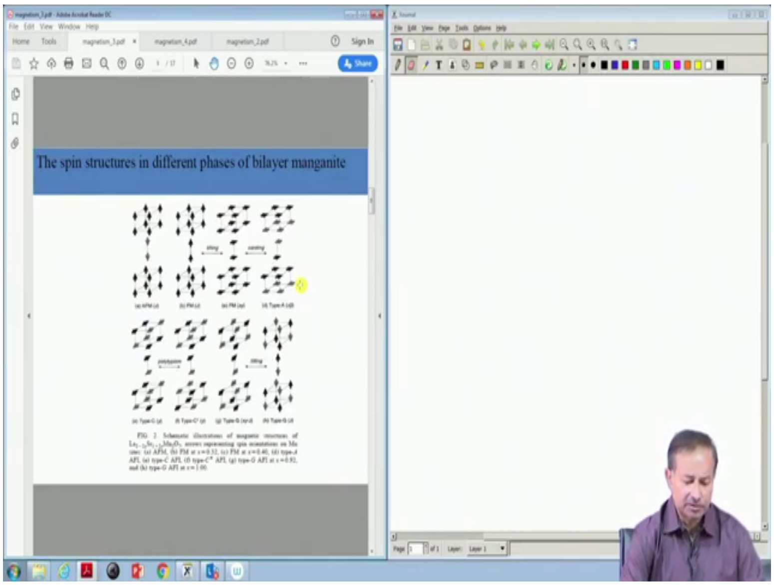

The spin structures in different phases of bilayer manganite

So, how do we find out these states; for example, this is another in bilayer manganites, these are complicated spin structures. So, there are two, perhaps two square, two cubes; one on top, one on below and in between there are two spins and these all these arranged in so many different ways.

And so, these are of course what nature gave us and these one has to understand these structures, starting from a microscopic theory. Ideally that is what the goal is and the scales involved in this; so one has to be able to predict the transition temperature, one should be able to tell us from the theory what kind of magnetic structure one should get into in the ground state and so on and so forth.

So, the, that is the role of the microscopic theory in this in all these magnetic systems. The interesting thing is how does one find out that such a, there are such complicated magnetic structures; well the standard experiment is that one does, a neutron scattering. So, that is something I will not discuss here, but that is an extremely powerful tool to find out the magnetic structure of a system.

Remember the overall moment or susceptibility will not give you the microscopic structure these details as; what is the direction of spin at each side, what is the magnitude of the moment at each side. So, in many systems of course, the atomic moment does not reflect into a in the actual moment, moments get reduced; so those are things that one has to understand and that comes from neutron scattering primarily. There are other experiments also which we will look at local magnetic environment and NMR, NQR these are some of the experiments; but this is the experimental details are extremely important and they are one independent course itself.

So, I will not get into those details, but remember the neutron scattering is one of the most favored method to and it is a very efficient method to find out the magnetic structure. And in India we of course, have such facility in BARC and the magnetic structure of materials can be determined by putting them under a neutron flux, which is obtained only in reactors, ok.

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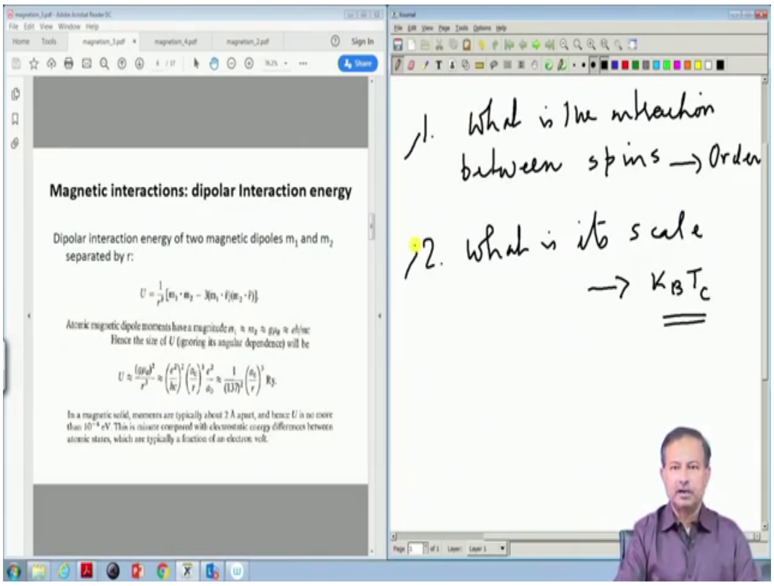

Magnetic interactions: dipolar Interaction energy

Dipolar interaction energy of two magnetic dipoles m_1 and m_2 separated by r:

$$U = \frac{1}{r^3}[\mathbf{m}_1 \cdot \mathbf{m}_2 - 3(\mathbf{m}_1 \cdot \hat{\mathbf{r}})(\mathbf{m}_2 \cdot \hat{\mathbf{r}})].$$

Atomic magnetic dipole moments have a magnitude $m_1 \approx m_2 \approx g\mu_B \approx e\hbar/mc$
Hence the size of U (ignoring its angular dependence) will be

$$U \approx \frac{(g\mu_B)^2}{r^3} \approx \left(\frac{e^2}{\hbar c}\right)^2 \left(\frac{a_0}{r}\right)^3 \frac{e^2}{a_0} \approx \frac{1}{(137)^2}\left(\frac{a_0}{r}\right)^3 \text{Ry}.$$

In a magnetic solid, moments are typically about 2 Å apart, and hence U is no more than 10^{-4} eV. This is minute compared with electrostatic energy differences between atomic states, which are typically a fraction of an electron volt.

1. What is the interaction between spins → Order

2. What is its scale → $K_B T_c$

So, so far so good, so I have raised a few things; one is that, that there are materials which are spontaneously ordered. Now, the question that I raised about them is that, there are they we need to know what orders them, what is the interaction between the moments that order them. Look at the situation, this is no longer a independent moment; each moment knows what the other moment is the direction of the other moment, that means there is a long range order.

For example, if you go back to these any of these pictures, not the first paramagnet, but the ordered ones ferromagnet or antiferromagnet and so on; if you know the spin of any at any moment anywhere in this, then you know the spins of every other moment.

So, supposing I know this bloop spin is up, then I can find out the moment of any other moment, any other find out the direction of any other moment anywhere in the lattice. And this is the macroscopic size and we are talking about an order which is far long in length scale than the size of atoms. So, you are talking about sometimes in centimeters and these are atoms of size angstrom.

So, if you know this moment at the level of angstrom, you can predict the moments everywhere in a length scale of centimeter. So, that is the remarkable situation to think of think about it; these are called long range orders, the range is all infinite for all practical purposes. And that requires an interaction inside the system to set it up and question is what is that interaction?

So, that is one question. So, question one is, what is the interaction between spins? I will keep on calling spins, but this is moments can be more than half and can be l plus s j and so on; but one generally refers to them all as spins in a magnetic system. It is a loose word; but it does not refer to only spin, but it refers to the moment.

And the, so what is the interaction between spins and one has to know how the spins talk to each other. Otherwise this long range order would not sit in, right. So, because they talk to each other; the moment one orders, they everybody else knows which way to point and that is like a talking to each other. So, that is the talking that we are talking we are discussing here and we need to find out that interaction, which causes all the spins to align in a particular way.

The other question is what is its scale? Now, in both these questions one and two we know the answer experimentally, although why we do not know the answer to question one experimentally; but we know the answer to one at least the nature of the ground state. So, we know whether it is a ferromagnet or an antiferromagnet or a ferromagnet a ferrimagnet or any other exotic order, any other complicated order, so, that is already given to us by experiment.

The second one of course is given to us by experiment as I said; the scale is the interaction scale is already set by the T C. So, T C is the K B T C is; so this one we already know that it is experimentally K B T C is the ordering energy, typical ballpark figure.

So, that is something we know and in this case we know the order the ground state, right the order. So, these are experimentally already determined; whereas we need to find out how these interactions come about, ok. So, so this question is to be answered first; if we know this, then we can answer the second, because then we already know the scale of this theory from microscopic.

Remember there are two ways to attack this problem; one is you just do the experiment and find out what is the situation, but then you need to know why is this situation there. And this why requires you to do a microscopic theory and develop a microscopic understanding of it and that is what our next step will be; I will argue as to from where does this interaction come and then what should be its scale.