Electronic Theory of Solids
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Lecture – 39
Magnetic Order

So, we have been discussing the Magnetic Interaction between Electrons in a solid for example. And what we have shown is that the way to go about is that you have to write a joint wave function. And that wave function, then you have to with that wave function you have to calculate the coulomb matrix element, the Hamiltonian matrix element in which there is a coulomb interaction as well.

And that matrix element is different for singlet and a triplet configuration, because your wave function has to be antisymmetrized. So, that antisymmetrization can be done in two ways; one is the symmetric wave function, another is the anti symmetric wave function.

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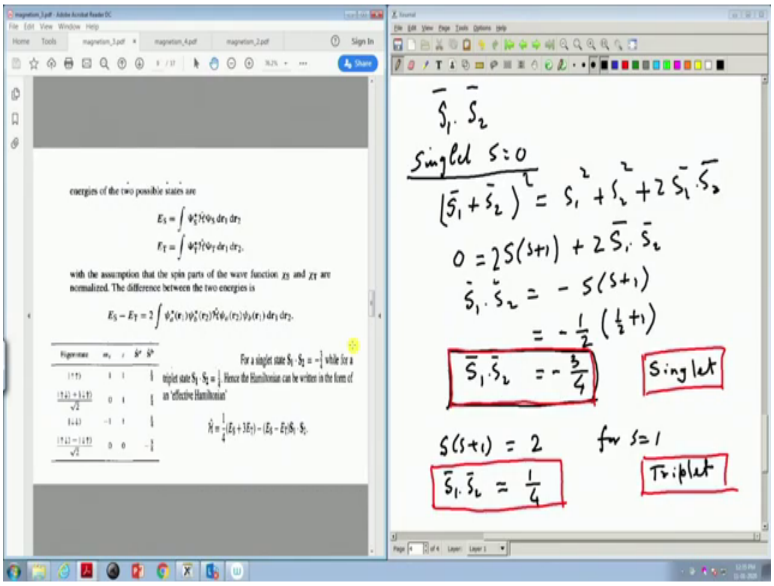

energies of the two possible states are

$$E_S = \int \Psi_S^* \hat{\mathcal{H}} \Psi_S \, d\mathbf{r}_1 \, d\mathbf{r}_2$$

$$E_T = \int \Psi_T^* \hat{\mathcal{H}} \Psi_T \, d\mathbf{r}_1 \, d\mathbf{r}_2,$$

with the assumption that the spin parts of the wave function χ_S and χ_T are normalized. The difference between the two energies is

$$E_S - E_T = 2 \int \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)\hat{\mathcal{H}}\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\, d\mathbf{r}_1 \, d\mathbf{r}_2.$$

Eigenstate	m_s	s	$\hat{S}^a \cdot \hat{S}^b$
$\|\uparrow\uparrow\rangle$	1	1	$\frac{1}{4}$
$\frac{\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle}{\sqrt{2}}$	0	1	$\frac{1}{4}$
$\|\downarrow\downarrow\rangle$	−1	1	$\frac{1}{4}$
$\frac{\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle}{\sqrt{2}}$	0	0	$-\frac{3}{4}$

For a singlet state $\mathbf{S}_1 \cdot \mathbf{S}_2 = -\frac{3}{4}$ while for a triplet state $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{4}$. Hence the Hamiltonian can be written in the form of an 'effective Hamiltonian'

$$\hat{\mathcal{H}} = \frac{1}{4}(E_S + 3E_T) - (E_S - E_T)\mathbf{S}_1 \cdot \mathbf{S}_2.$$

$\bar{S}_1 \cdot \bar{S}_2$

Singled $S = 0$

$(\bar{S}_1 + \bar{S}_2)^2 = S_1^2 + S_2^2 + 2\bar{S}_1 \cdot \bar{S}_2$

$0 = 2S(S+1) + 2\bar{S}_1 \cdot \bar{S}_2$

$\bar{S}_1 \cdot \bar{S}_2 = -S(S+1)$

$= -\frac{1}{2}\left(\frac{1}{2}+1\right)$

$\boxed{\bar{S}_1 \cdot \bar{S}_2 = -\frac{3}{4}}$ $\boxed{\text{Singlet}}$

$S(S+1) = 2$ for $S = 1$

$\boxed{\bar{S}_1 \cdot \bar{S}_2 = \frac{1}{4}}$ $\boxed{\text{Triplet}}$

And these are basically their spin states are correspondingly singlet and triplet and these states when you take a when you calculate the energy difference between the singlet and the triplet in such a state such states then you will find that it is non zero. And that means, the although coulomb interaction does not care about the moments the antisymmetrization brings in a spin dependent term in the energies and; that means, the triplet we where the two spins are either up or down; that means, they are parallel is different the energy of that is different from the energy where the two spins are anti parallel.

So, that is a really remarkable result coming out of quantum mechanics and what we will do is, now using that try to write down a Hamiltonian which describes these spin interaction. So, we will not bother about charges because these are mostly magnetic insulators not iron cobalt nickel, but many of these materials are magnetic insulators and their moments are basically sitting tightly in their with their atoms.

And therefore, charge degree of freedom movement of charge is already quenched. So, the only degree of freedom left is their spins and we know that they are magnetically ordered and so, therefore, we know that the spins are talking to each other. And so, the dominant part of the Hamiltonian for in these cases is coming from the magnetic interaction.

And that is the interesting part because we want to also find out the magnetic state of the system so, that is the Hamiltonian that we are going to write. So, it is a spin Hamiltonian where charge degrees are we are not even bothered about and in insulator of course, the charge degree of freedom is mostly irrelevant for the description of dynamics or the low lying excitations of a system.

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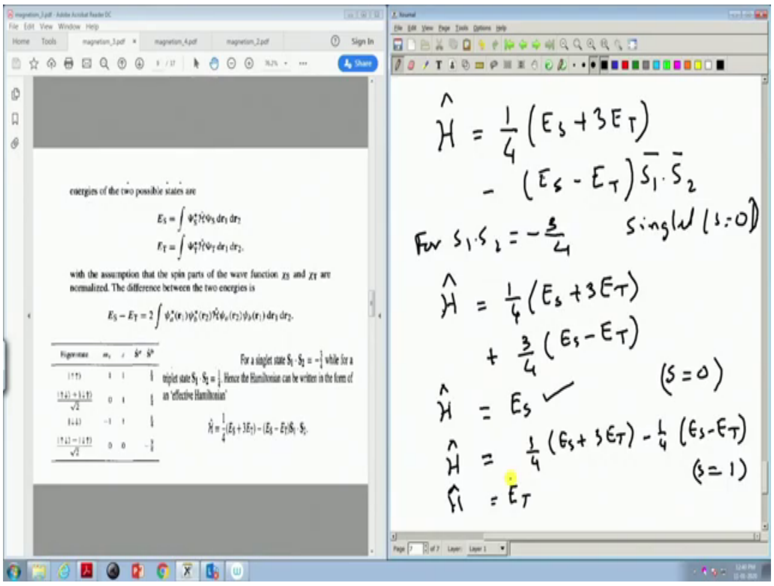

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For $S_1 \cdot S_2 = -\frac{3}{4}$ singlet $(s=0)$

$$\hat{\mathcal{H}} = \frac{1}{4}(E_S + 3E_T) + \frac{3}{4}(E_S - E_T)$$

$$\hat{\mathcal{H}} = E_S \checkmark \qquad (S=0)$$

$$\hat{\mathcal{H}} = \frac{1}{4}(E_S + 3E_T) - \frac{1}{4}(E_S - E_T) \qquad (S=1)$$

$$\hat{\mathcal{H}} = E_T$$

So, let us go ahead and write this formula E S plus. So, the claim is that we can write a Hamiltonian, which is put a hat Hamiltonian operator in terms of this these differences in energies E S plus 3 E T minus E S minus E T S 1 dot S 2. S 1 and S 2 are these two spins we are we are discussing of the two electrons ok. So, let us put the E S the value S 1 dot S 2 in the two cases. So, for S 1 dot S 2 equal to minus 3 by 4 which is singlet total S 0 this let us calculate it. So, H will be H will give me one - fourth E S plus 3 E T minus plus three - fourth E S minus E T.

So, this is one - fourth plus three-fourth is 1 E S and this is three-fourth minus three-fourth is 0. So, this is E S. So, that is so, for singlet total spin S equal to 0 it is giving me the correct energy which is E S ok. Similarly you do it for H for triplet, equal to that is one – fourth so, one-fourth E S plus 3 E T minus one-fourth E S minus E T. So, this is S equal to 1 and just you can immediately see that this gives me back E T.

So, this Hamiltonian the way it is written is correctly reproducing the two cases, for S equal to 0 it is giving me E S, for S equal to 1 it is giving me E T. So, this is a right form of the Hamiltonian.

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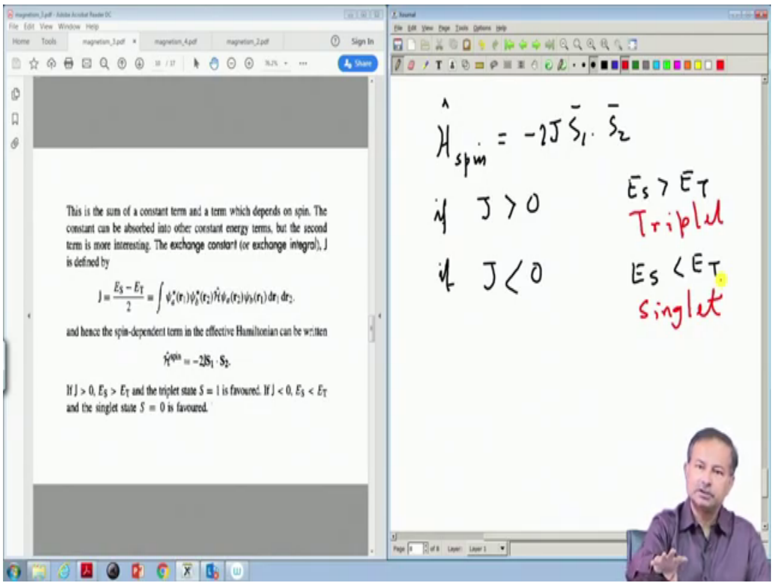

This is the sum of a constant term and a term which depends on spin. The constant can be absorbed into other constant energy terms, but the second term is more interesting. The **exchange constant** (or **exchange integral**), J is defined by

$$J = \frac{E_S - E_T}{2} = \int \psi_a^*(\mathbf{r}_1)\psi_b^*(\mathbf{r}_2)\hat{\mathcal{H}}\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)\,d\mathbf{r}_1\,d\mathbf{r}_2.$$

and hence the spin-dependent term in the effective Hamiltonian can be written

$$\hat{\mathcal{H}}^{\text{spin}} = -2J\mathbf{S}_1 \cdot \mathbf{S}_2.$$

If $J > 0$, $E_S > E_T$ and the triplet state $S = 1$ is favoured. If $J < 0$, $E_S < E_T$ and the singlet state $S = 0$ is favoured.

$$\hat{H}_{spin} = -2J\bar{S}_1 \cdot \bar{S}_2$$

if $J > 0$ $E_S > E_T$ Triplet

if $J < 0$ $E_S < E_T$ Singlet

Now, the first term is of course, you in a in a any Hamiltonian if there is a constant energy there is no operator here there is no spin operators in the first term these are just to sum of two constants E S and E T just numbers. So, you can just absorb it into your 0 of energy you can set your 0 there. So, other the other constant terms in there are lots of other energies that come in the system. So, all that constant energies can always be sort of absorbed in those. So, second term is the one which is which carries an operator product of two operators S 1 and S 2 and that contains this E S minus E T.

Now E S minus E T by 2 is generally referred to as J and it is called the exchange constant, this is the magnitude of the exchange interaction just divided by 2 and so, that gives me a. So, that is that I can write a spin dependent term part of the Hamiltonian which is what I am interested in which is H spin equal to minus 2 J S 1 dot S 2 even the J is E S minus E T by 2. So, then you can see immediately that if J if J equal to J greater than 0, which means E S is greater than E T then the S equal to then the two spins will try to align because there is a minus sign outside J is greater than 0. So, if the two spins align in the same direction the energy will be lower so, you will get the triplet. So, this will lead to a triplet state immediately.

On the other hand if J is if J is negative, then this term becomes now positive and then S 1 and S 2 then we will try to misalign they will just be anti parallel. So, that this becomes negative. So, you will get a single. So, here you have E S less than E T and therefore, E S is a S is the state where it will go singlet, because that is the lower energy and that is exactly what we are finding.

So, that tells us that this Hamiltonian actually represents the correct physical picture when spin interactions are concerned. So, this is the spin Hamiltonian this is the one that we should be using to understand everything that happens for the magnetic state of the system. So, that is that is exactly what is saying this is this is the spin Hamiltonian, you can go to many much larger systems.

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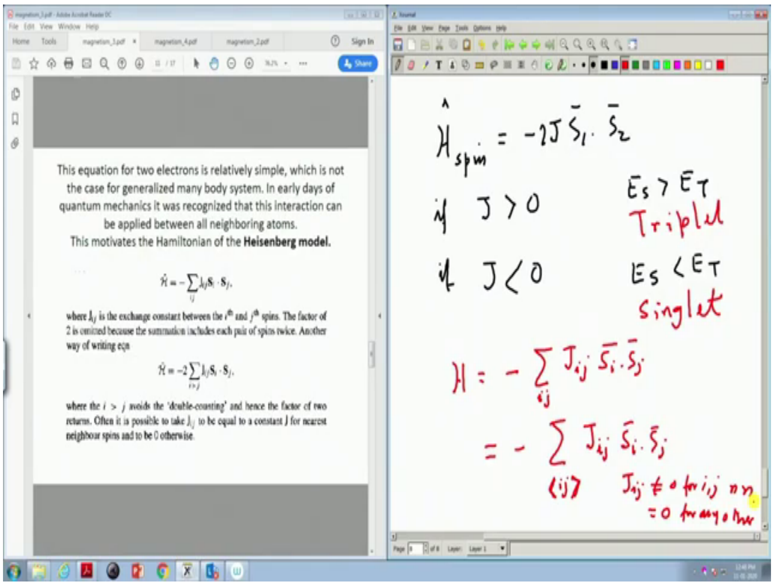

This equation for two electrons is relatively simple, which is not the case for generalized many body system. In early days of quantum mechanics it was recognized that this interaction can be applied between all neighboring atoms.

This motivates the Hamiltonian of the **Heisenberg model.**

$$\hat{\mathcal{H}} = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j,$$

where J_{ij} is the exchange constant between the i^{th} and j^{th} spins. The factor of 2 is omitted because the summation includes each pair of spins twice. Another way of writing eqn

$$\hat{\mathcal{H}} = -2\sum_{i>j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j,$$

where the $i > j$ avoids the 'double-counting' and hence the factor of two returns. Often it is possible to take J_{ij} to be equal to a constant J for nearest neighbour spins and to be 0 otherwise.

$$\hat{H}_{spin} = -2J\bar{S}_1 \cdot \bar{S}_2$$

if $J > 0$ $E_S > E_T$ Triplet

if $J < 0$ $E_S < E_T$ Singlet

$$H = -\sum_{ij} J_{ij}\bar{S}_i \cdot \bar{S}_j$$

$$= -\sum_{\langle ij \rangle} J_{ij}\bar{S}_i \cdot \bar{S}_j$$

$J_{ij} \neq 0$ for i, j nn

$= 0$ for any other

For two electrons is very simple generally in many body system of course, it is much more complicated, but still one has two one uses this because this is this is motivated by very simple calculations and simple arguments and in many cases it actually works. And so, what one writes for a multi electron for the many body system is still a Hamiltonian of this type, where you use this S 1 dot S 2 now this S 1 dot S 2 S 1 dot S 3 S 2 dot S 3 S 2 dot S 4 S 1 dot S 4 for all come possible pair wise interaction between spins. So, that is the interesting part that one is not considering multi spin interaction S 1 S 2 S 3 S 1 S 2 S 5 and so on and so forth. So, those are not being considered.

So, simple model was written down by Heisenberg which is this famous model called Heisenberg model J ij S i dot S j, where i and j are the side indices or the spins where basically the spins at this i th side and j th side. So, and their interaction between them is J ij, you remember that this J ij still arbitrary we have to determine it from system to system. For example, in a in a for example, if we know the system is ferromagnetic then we know that all these Js are greater than 0, because then you have all spins all S i's and S j's are aligned in the same direction to minimize the energy, that would be the preferred directions.

Whereas, if they are this is negative then of course, the situation can be complicated because spin 1 interacts with 2, then spin 1 also interacts with 3 and in that case for example, spin 1 will like 2 and 3 both to be anti parallel with itself; whereas, spin 2 and 3 will also want to be anti parallel with itself because of this if J ijs are all negative. So, that is that brings in complications in the system ferromagnetism is therefore, much easier to understand.

Nevertheless, the there is a simpler version of this in this Hamiltonian where one assumes that the moments of a particular site of any site the moment is talking only to it is nearest neighbors. The interaction with the next nearest neighbor is much weaker; because the overlap of the wave function the matrix element requires you to calculate the wave function at this side matrix element the Hamiltonian with the wave function at the other side.

So, that is much weaker if you go beyond the first neighbor your nearest neighbor. So, in that case one is one writes a Hamiltonian, which is called the nearest neighbor Heisenberg Hamiltonian and that is the one which is mostly used J ij S i dot S j, this the sign at the summation index refers to the fact that you are only calculate considering J ij equal to J ij nonzero for ij nearest neighbor and 0 for any other, ok. So, that is called nearest neighbor Heisenberg model; that is the most common model that one studies.

Now the thing is that if you if you just look at just for the sake of bookkeeping one has to remember that the way I have written here is i and j are unrestricted summation. So, i can take one j can also take one at some point. So, of course, the interaction between spins at the same site is basically you do not consider that that is not there is only one moment sitting at each side. So, i equal to j is not the interesting part, but i and j take all values right. So, i equal to j is basically 0. So, you do not bother about that, but i not here i is i can take a value which j can also take at some point.

For example, the bond the J ij s are defined on a bond right; because it is ij 1 2, 2 3, 3 4 and so on. So, this is between in between the two spins which means there is a bond. So, that bond is counted twice here because 1 2 and 2 1 will both be counted if I sum unrestricted sum of J ij. So, that can be prevented by a method in which you just keep i greater than j for example. So, in that case you will have twice the factor because here you had each bond counted twice. So, here you are counting once so, that is the factor of 2.

So, that is, but these are just bookkeeping one as long as you know what you are doing you do not have to bother, the second convention is not very common and the first one is the one writes. So, the nearest neighbor as said often it is possible to take J ij to be equal to a constant

J. So, you can actually replace this by a constant and only then take J out and S i dot S j. And then consider only also consider only the nearest neighbors so, ij.

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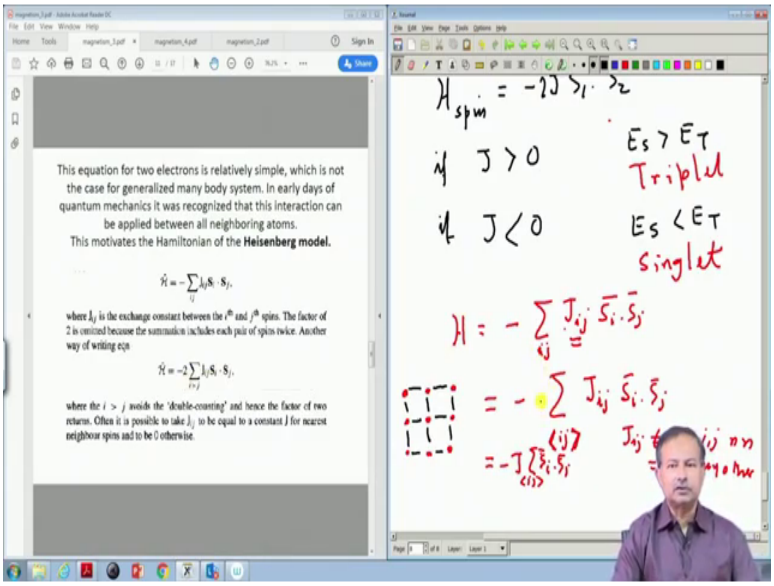

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$$H_{spin} = -2J S_1 \cdot S_2$$

if $J > 0$ $\quad E_S > E_T$ Triplet

if $J < 0$ $\quad E_S < E_T$ singlet

$$H = -\sum_{ij} \underline{\underline{J_{ij}}} \bar{S}_i \cdot \bar{S}_j$$

$$= -\sum_{\langle ij \rangle} J_{ij} \bar{S}_i \cdot \bar{S}_j$$

$$= -J \sum_{\langle ij \rangle} \bar{S}_i \cdot \bar{S}_j$$

J_{ij} ij nn

otherwise

So, this is how you write. So, S j minus J S i dot S j i and ij are nearest neighbors and J is a fixed constant between any two bonds. So, the J's are basically suppose these are your sites where spins are sitting and J's are then defined over the bonds. So, J ij j 1 2 for example, will be this between is we can write it this way these are the j 1 2's and all these are taken to be the same for in this model.

There are models where these J ij's differ between bonds they can be random they can be plus or minus and so on and so forth. But for the standard models of ferromagnetism and anti ferromagnetism these values of j are fixed between nearest neighbor and beyond nearest neighbor you do not consider the interaction J ij is considered to be 0. So, that is the simplest model one can study, but certainly it is an approximation, but it works fairly well for most systems that we study.

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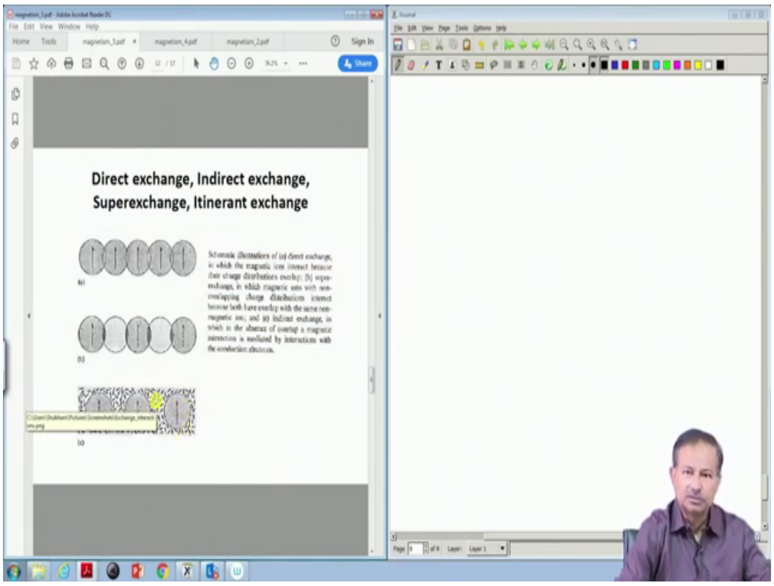

Direct exchange, Indirect exchange, Superexchange, Itinerant exchange

Schematic illustrations of (a) direct exchange, in which the magnetic ions interact because their charge distributions overlap; (b) superexchange, in which magnetic ions with non-overlapping charge distributions interact because both have overlap with the same non-magnetic ion; and (c) indirect exchange, in which in the absence of overlap a magnetic interaction is mediated by interactions with the conduction electrons.

So, these exchange can of course, be of various types some are discussed here. In books you will find that there are many exchanges that I discussed direct exchange, indirect exchange, super exchange, itinerant exchange and so on and so forth. So, let me just outline a few this is for example, a direct exchange where the two spins are sitting next to each other and they are talking to each other their wave functions can overlap.

And the matrix element of H between them is what you calculate for exchange. So, this is called the direct exchange, but it can also happen that there is a non magnetic iron sitting in between the two spins. So, in that case these these moments talk to the next moment via this non magnetic iron ok. So, these magnetic ions do not overlap their wave functions do not overlap. Whereas the non magnetic ion is with which it they overlap and why are these non magnetic ion they can interact with each other that is an indirect exchange it is also called super exchange.

So, there is another kind of interaction which is mediated by the intervening interactions with the conduction electrons. So, this moment for example, is far from this moment fairly away from this next moment which is again fairly away from this moment. But, this moment talks to the conduction electrons nearby polarizes them and that polarization can carry the information of the magnetic history of this ion to the next one and then that sets of an effective interaction magnetic interaction between this ion and that ion. So, that is that is another indirect exchange in which the conduction electron plays a role.

So, the magnet here the magnetic ions are separated they are deep lying states with magnetic moments. And there is a conduction band above it they these deep lying moments for example, for f moments in rare earths and they talk to the magnetic to the to the conduction electrons and interact with the conduction electrons polarizes them the conduction electrons that polarization then goes to the next deep lying moment.

And then passes on the history on that information to the next ion and that is that can set up an interaction between these two. So, this is fairly indirect mediated by conduction electrons which are different and, but this happens and this is found out is a very famous example and as I we discussed in GMR for example, this is used to set up this magnetic interaction between the layers.

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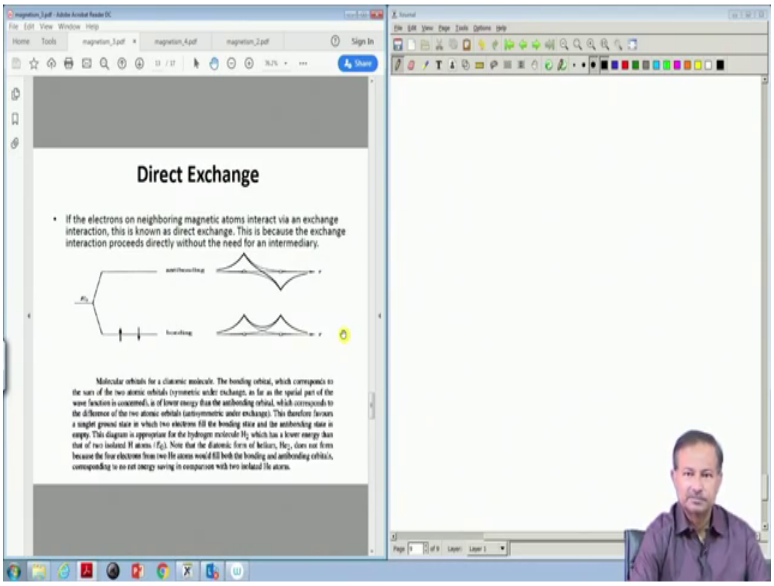

Direct Exchange

- If the electrons on neighboring magnetic atoms interact via an exchange interaction, this is known as direct exchange. This is because the exchange interaction proceeds directly without the need for an intermediary.

Molecular orbitals for a diatomic molecule. The bonding orbital, which corresponds to the sum of the two atomic orbitals (symmetric under exchange, as far as the spatial part of the wave function is concerned), is of lower energy than the antibonding orbital, which corresponds to the difference of the two atomic orbitals (antisymmetric under exchange). This therefore favours a singlet ground state in which two electrons fill the bonding state and the antibonding state is empty. This diagram is appropriate for the hydrogen molecule H_2 which has a lower energy than that of two isolated H atoms (E_0). Note that the diatomic form of helium, He_2, does not form because the four electrons from two He atoms would fill both the bonding and antibonding orbitals, corresponding to no net energy saving in comparison with two isolated He atoms.

So, this direct exchange is something that we have actually done when we did this hydrogen molecule theory remember we calculated the two states which were bonding and anti bonding. So, look at the situation there remember that when two protons with their electrons hydrogen atoms came close and they basically started talking to each other.

Now this talking at that point we did not bothered about the magnetic part of it, but I just mentioned passingly that the state that it goes to has no spin it is a singlet state. So, that is an interesting observation and that we I postponed that discussion till here, because now we are doing magnetism. And now you see what is happening these two spins of the to the two electrons which are far apart initially they were independent, they could point in any direction which is like a paramagnet.

But when they came close by they started talking to each other and they form these two levels, which are bonding and anti bonding and we have to put two electrons. And we can do it and we will do it in such a way that we have already done that we put two electrons at the lower and lower bonding orbital to gain the energy. And that energy gain gives us a magnetic state, which is already which gets fixed the magnetic state is a singlet, because you are putting two electrons in the same bonding orbital.

So, that you have to be a in a singlet state by Pauli principle the spins have to be up and down. So, the so, that means, that in hydrogen molecule for example, where we discuss two electron problem we actually have a magnetic order which is it is not the magnetic order, but the magnetic state is fixed. So, the state is a singlet one spin up, the other has to be down.

Of course in helium as we as you remember we could not do it we do not do this because helium will also have this other two electrons we have to put in no energy is gained. So, it does not form that molecule, but that is a different matter. But this is a direct exchange example of a direct exchange between when a hydrogen molecule forms or when two hydrogen atoms come very close to each other, their spins lock into a singlet state which is magnetic in the sense it is a singlet magnetic state, it does not have access to the triplet state. So, if you measure spin you will find 0 moment is 0.

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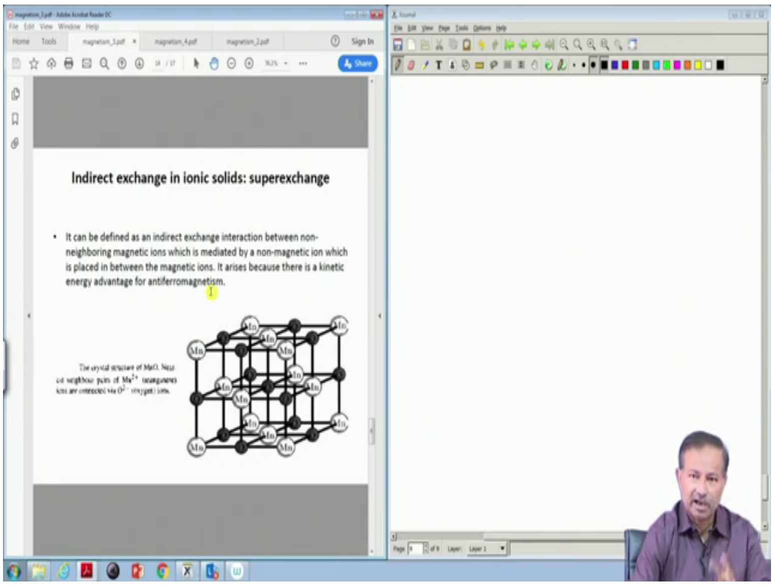

Indirect exchange in ionic solids: superexchange

- It can be defined as an indirect exchange interaction between non-neighboring magnetic ions which is mediated by a non-magnetic ion which is placed in between the magnetic ions. It arises because there is a kinetic energy advantage for antiferromagnetism.

The crystal structure of MnO. Nearest neighbour pairs of Mn^{2+} (manganese) ions are connected via O^{2-} (oxygen) ions.

So, in ionic solids for example, the super exchange that I just described you via a intervening non magnetic ion you can have although the two moments wave functions two electrons wave functions do not overlap. They can interact via a non magnetic ion sitting in between that non magnetic iron in most cases in many cases is an oxygen, oxygen O 2 minus which has a completely filled shell. So, that becomes non magnetic and this is an example for a in M n O see the O 2 minus are these dark circles and 2 M n's are far a quite I mean they are not near next to each other.

There is an oxygen atom between any two M n in this M n O, but this M n and that M n actually talked to each other and that is why are this oxygen. And that is called the called a super exchange and that comes from the from kinetic energy that one gains by delocalizing which is again the Heisenberg uncertainty also tells us the same thing that. If you delocalize you gain energy the electrons have kinetic energy now.

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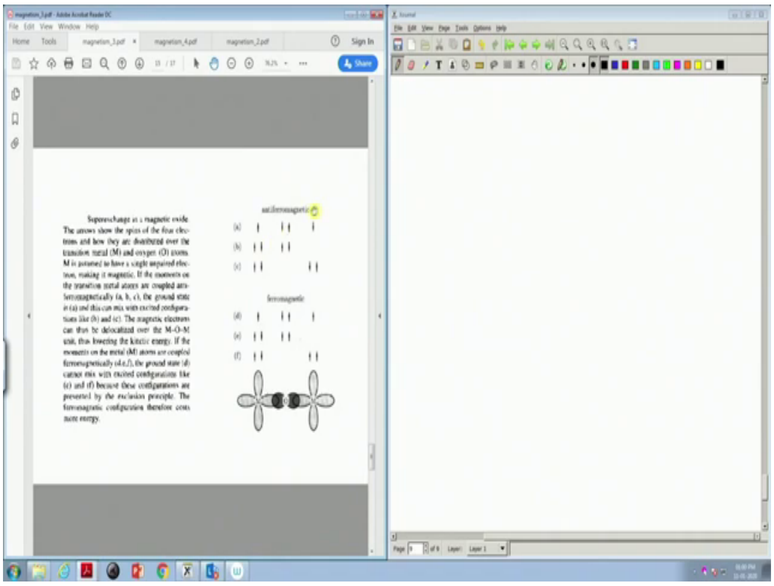

Superexchange in a magnetic oxide. The arrows show the spins of the four electrons and how they are distributed over the transition metal (M) and oxygen (O) atoms. M is assumed to have a single unpaired electron, making it magnetic. If the moments on the transition metal atoms are coupled antiferromagnetically (a, b, c), the ground state is (a) and this can mix with excited configurations like (b) and (c). The magnetic electrons can thus be delocalized over the M-O-M unit, thus lowering the kinetic energy. If the moments on the metal (M) atoms are coupled ferromagnetically (d,e,f), the ground state (d) cannot mix with excited configurations like (e) and (f) because these configurations are prevented by the exclusion principle. The ferromagnetic configuration therefore costs more energy.

So, here is a simple way of showing it more or less a cartoon way of showing it, this is anti ferromagnetic arrangement and this is a ferromagnetic arrangement. And you can work it out yourself it is all written on the left what you have to do, you have to you have to see that you see that the a is the is a configuration that you have chosen where the interaction is anti ferromagnetic.

So, this electron in manganese and this electron in the next manganese are anti ferromagnetically coupled and there is a oxygen with the states is completely filled up. So, they this is completely filled two electrons are already there it is non magnetic. In this case you can go to the excited states quite easily, you can do it yourself you can see clearly that you can exchange this you can move this electron here and this electron the right electron here and you can go to a.

For example, what has been done here is, this down electron from here has been moved here in b. So, we are left with an up electron then you can move the down electron from here and up down here and none here nothing here. So, in effect what you have done is transferred an electron from right which is down spin to extreme left right in effect that is what is happened.

That means you this electron the right got gained a kinetic energy similar things can be done in c where you can actually delocalize the oxygen’s two electrons on to the near neighboring manganese sides. There is a lot of delocalization energy that you gain here, the electrons can move and then that is called delocalization and that gives you energy.

Whereas this d state which is the same configuration, but we have now they have now put ferromagnetical interaction between this they are assuming a ferromagnetic interaction between this manganese and this manganese. And in this ferromagnetic configuration you can easily work out you can I leave it to you to do it, you can see that this e and f states which are the where you can delocalize you are they are not accessible to it cannot do it.

The ground state d cannot mix with excited configurations likes e and f, because these configurations are prevented by Pauli principle ok. So, you cannot go from d to e or f that is what is called mixing; I mean the quantum mechanics you get a mixed states the overlap is non zero between these two states. So, that is an example where the anti ferromagnetic arrangement will be favored than the ferromagnetic arrangement of the manganese beams. So, this spin and this spin being ferromagnet is a bad choice this being anti ferromagnet is a better much better choice.

Where you electron can delocalize and gain a lot of energy. So, that is what one that is the super exchange mechanism, it is it leads to anti ferromagnetism in this kind of a configuration, where an oxygen atom is on both sides of it the manganese spin of manganese for example, is sitting.

And of course, this is and this is the straight line arrangement. There are different arrangements where this manganese on the left can be on top and there of course, the interactions might become different. But in this arrangement this is an is a simple example on a linear chain you can see that the anti ferromagnetic state is favored over the ferromagnetic state simply by gaining kinetic energy it can lower it is energy.

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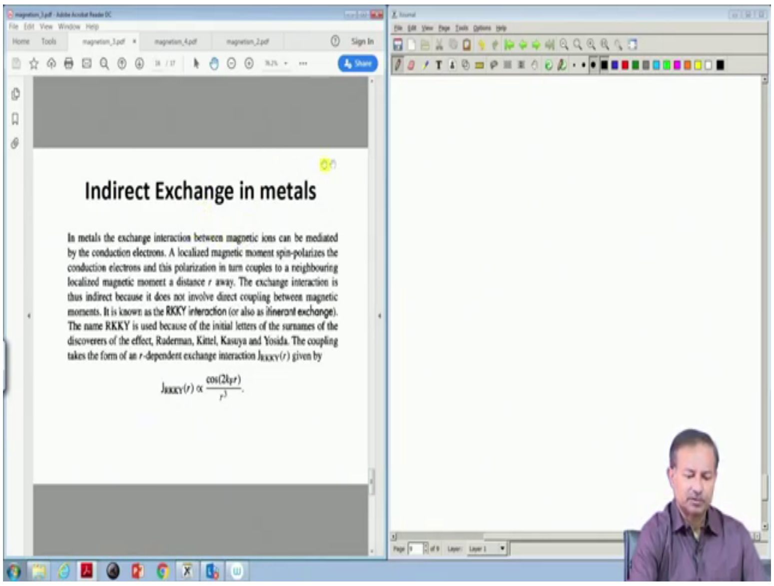

Indirect Exchange in metals

In metals the exchange interaction between magnetic ions can be mediated by the conduction electrons. A localized magnetic moment spin-polarizes the conduction electrons and this polarization in turn couples to a neighbouring localized magnetic moment a distance r away. The exchange interaction is thus indirect because it does not involve direct coupling between magnetic moments. It is known as the **RKKY interaction** (or also as **itinerant exchange**). The name RKKY is used because of the initial letters of the surnames of the discoverers of the effect, Ruderman, Kittel, Kasuya and Yosida. The coupling takes the form of an r-dependent exchange interaction $J_{RKKY}(r)$ given by

$$J_{RKKY}(r) \propto \frac{\cos(2k_F r)}{r^3}.$$

So, these are example of different kinds of exchanges. We will come to indirect exchange and just discuss one or two more examples in the next class and then carry on working with this Heisenberg model and it is different versions different incarnations and in different situations.