Condensed Matter Physics
Prof. G. Rangarajan
Department of Physics
Indian Institute of Technology, Madras

Lecture - 22
Exchange Interactions, Magnetic Order Neutron Diffraction

In the last lecture, we saw briefly the mechanism or the interaction which is basically responsible for ferromagnetic ordering. In a magnetic solid, we said that this interaction is known as the exchange interaction and also indicated that to understand the how this exchange interaction works. It is necessary to consider the so called Heitler-London model of a homonuclear diatomic molecule such as hydrogen.

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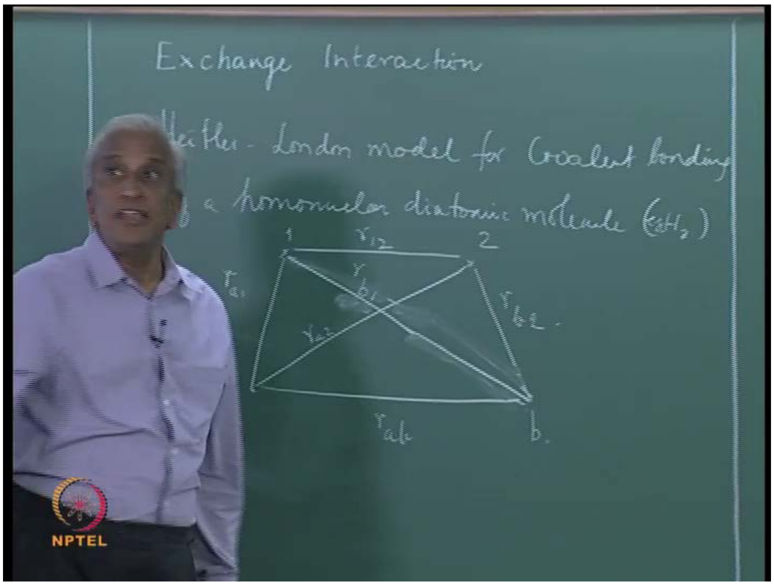

So, in this lecture, we will consider this in greater detail. So, we will be discussing exchange interaction using the Heitler-London model for covalent bonding of a homoneuclar diatomic molecule such as hydrogen example. So, we already started and this for today we will talk a little bit in greater detail on this.

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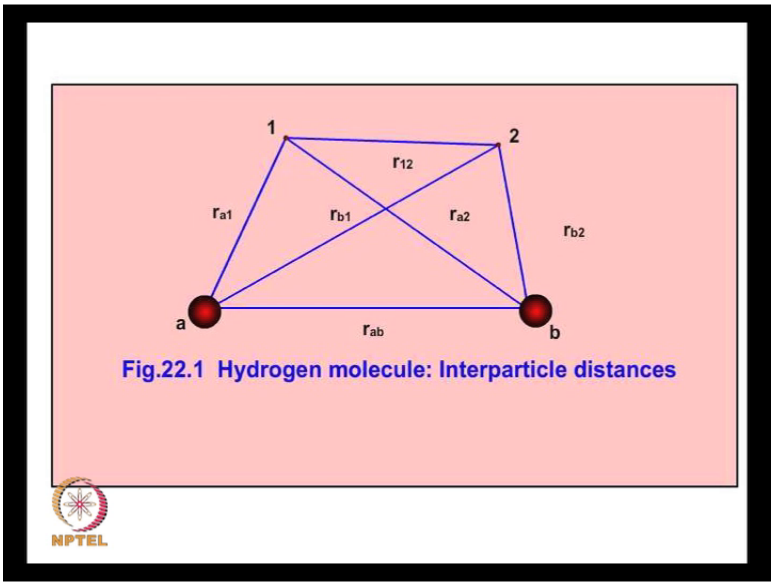

Fig.22.1 Hydrogen molecule: Interparticle distances

So, the figure shows the hydrogen molecule and you have the two nuclei a and b are the atomic nuclei of the hydrogen atom which are represented by well. These are the nuclei and then you have the electrons 1 and two the hydrogen has 2 atomic nuclei and two electrons. So, nuclei are shown by the letters a and b and the electrons are indicated by the numbers 1 and two. So, the various distances are this is r a 1, this is r b 2 this is r a 2 this is this is r a 2 this is r b 1 we also have r 1 2 and we have r a b, these are the various distances.

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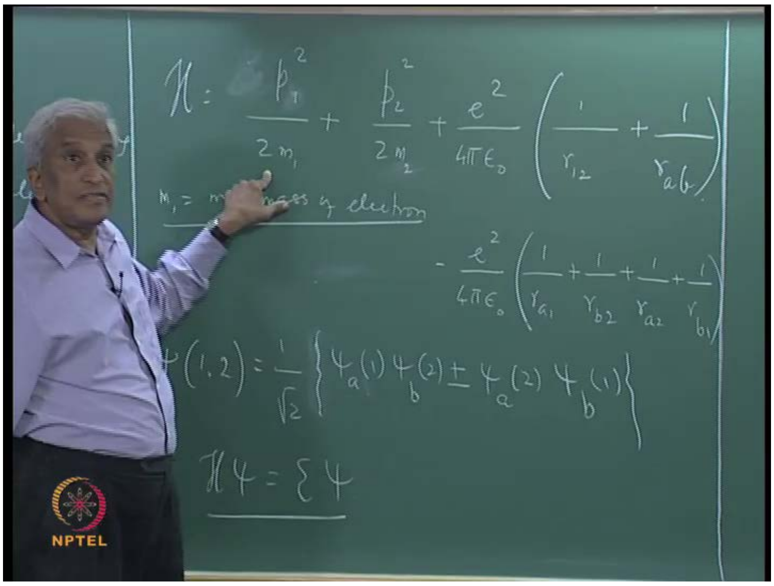

$$\mathcal{H} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{12}} + \frac{1}{r_{ab}}\right)$$

$m_1 = m$ mass of electron

$$- \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{a1}} + \frac{1}{r_{b2}} + \frac{1}{r_{a2}} + \frac{1}{r_{b1}}\right)$$

$$\psi(1,2) = \frac{1}{\sqrt{2}}\left\{\psi_a(1)\psi_b(2) \pm \psi_a(2)\psi_b(1)\right\}$$

$$\mathcal{H}\psi = E\psi$$

So, in terms of these distances, we can drive the Hamiltonian operator, the Hamiltonian operator will involve the individual kinetic energies of the two atoms e 1 square by 2 m plus p 2 square by 2 m where m is the mass of the electron. And you can say, 2 m 2, but this m 1 equal to m 2 equal to m e mass of electron. The electrons are identical and have the same mass then you have these square by 4 pi epsilon nought into 1 by r 1 2 plus 1 by r a b this is the repulsive energy potential energy of the two electrons and this is the repulsive potential energy of the two atomic nuclei. So, this a total repulsive potential energy term then you have binding or attractive terms potential energy terms due to the various interactions re 1 r p 2 1 by re 2 plus 1 by r b 1 these are the 4 interactions terms which constitute attractive potential energy terms. So, that is the total Hamiltonian of the two electron hydrogen molecule.

So, this is the Hamiltonian and we have to use the corresponding two electron wave functions which are at the form psi 1 2 equals 1 over root 2 which is a normalization constant time psi a 1 psi b 2 plus or minus psi a 2 psi b 1. So, that is the two electron wave function which involves the product wave functions. So, the single electron wave functions of the form psi a 1 and psi b 2 which means electron one is with the nucleus of the atom a and the electron two is with the nucleus b and, but it is also equally probable that the electron two spends time with the nucleus a while the electron one spends time with the nucleus b. So, both are equally probable and therefore, we put a linear combination of these two product wave functions this linear combination can be symmetric or anti symmetric with respect to a change of the electrons.

And therefore, the plus sign corresponds to the symmetric linear combination and the minus sign corresponds to an anti- symmetric linear combination both will give rise to the same modular square of the wave function and therefore, are equally probable. So, we had to consider both possibilities and this is the wave function which has to be combined with this in the solution of the Schrodinger equation of the form xi equal to psi where e is the energy Eigen value. So, we have to determine the energy Eigen values of the homonuclear diatomic molecule which has a Hamiltonian of this form and a wave function of this form. So, if we solve this problem and find the energy Eigen values we will have a clue to see which are the ground state energy what is the ground state energy which are the energetically favoured states of the molecule. So, this is the key to the entire question. So, when this is done.

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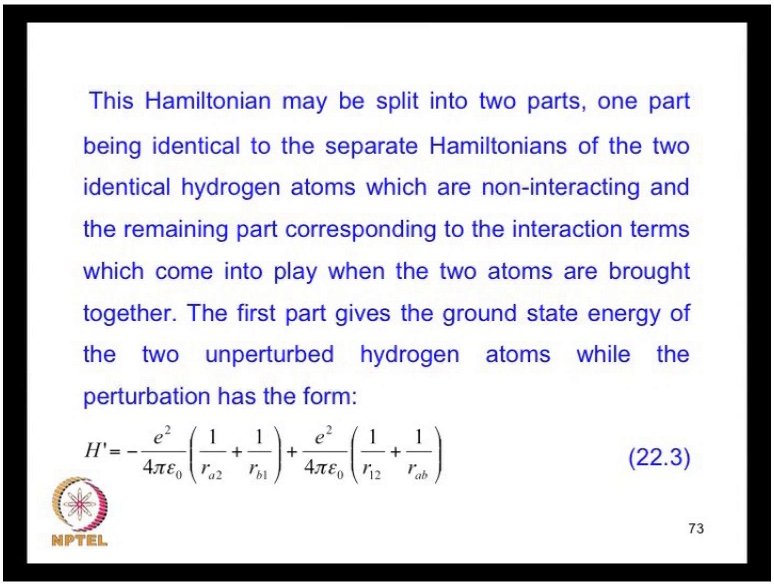

This Hamiltonian may be split into two parts, one part being identical to the separate Hamiltonians of the two identical hydrogen atoms which are non-interacting and the remaining part corresponding to the interaction terms which come into play when the two atoms are brought together. The first part gives the ground state energy of the two unperturbed hydrogen atoms while the perturbation has the form:

$$H' = -\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{a2}} + \frac{1}{r_{b1}}\right) + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_{12}} + \frac{1}{r_{ab}}\right) \qquad (22.3)$$

We see that if I have only the first part that is the we already know p one square by 2 m 1 minus e square by 4 pi epsilon naught r a 1. This is the potential energy term and this is the kinetic energy term of the hydrogen atom one. Similarly p 2 square by 2 m two with a minus e square by 4 pi epsilon nought one by r b 2 gives you the kinetic and potential energy terms of the Hamiltonian of the individual hydrogen atom two. So, these gives you the total energy this these two plus this 2 give you the energy Hamiltonian unperturbed terms of the Hamiltonian which corresponds to the total of which gives you the total energy of two unperturbed hydrogen atoms. So, the remaining terms or perturbations. So, this 1 is a perturbation and similarly these two terms are perturbation.

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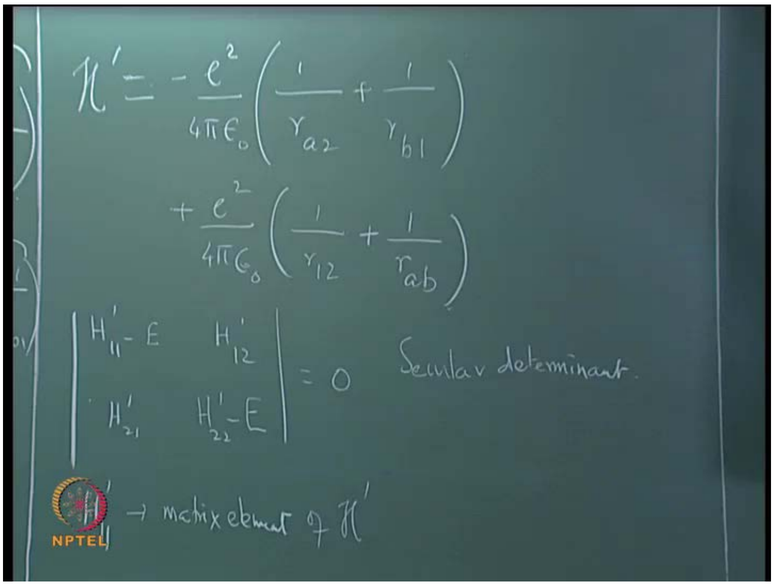

$$\mathcal{H}' = -\frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{a2}}+\frac{1}{r_{b1}}\right) + \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}\right)$$

$$\begin{vmatrix} H'_{11}-E & H'_{12} \\ H'_{21} & H'_{22}-E \end{vmatrix} = 0$$ Secular determinant.

H'_{11} → matrix element of $\mathcal{H}'$

These are extra terms. So, the perturbing Hamiltonian is of the form minus e square by by 4 pi epsilon nought times 1 by r a 2 plus 1 by r b 1 plus e square by 4 pi epsilon nought into 1 by r 1 2 is inter electron repulsion plus 1 by r a b which is the inter nuclear repulsion. So, these are the terms so the original unperturbed Hamiltonian has gives you the total energy the sum of the individual energies of the two isolated hydrogen atoms in their ground states, and but these extra terms in the un perturbing Hamiltonian modify this energy of the two electron Eigen function.

And these energy Eigen values in the presence of the perturbation are formed by solving the secular determinant according to perturbation theory which has the form H 1 1 prime minus E H 1 2 prime H 2 1 prime H 2 2 prime minus E equal to 0 that is known as the secular determinant. Here H 1 1 prime is the so called matrix element matrix element of the perturbing Hamiltonian H prime with between the states I one and psi 1. So, we have similarly H 1 2 prime is the matrix element between the states psi 1 and psi 2 and so on.

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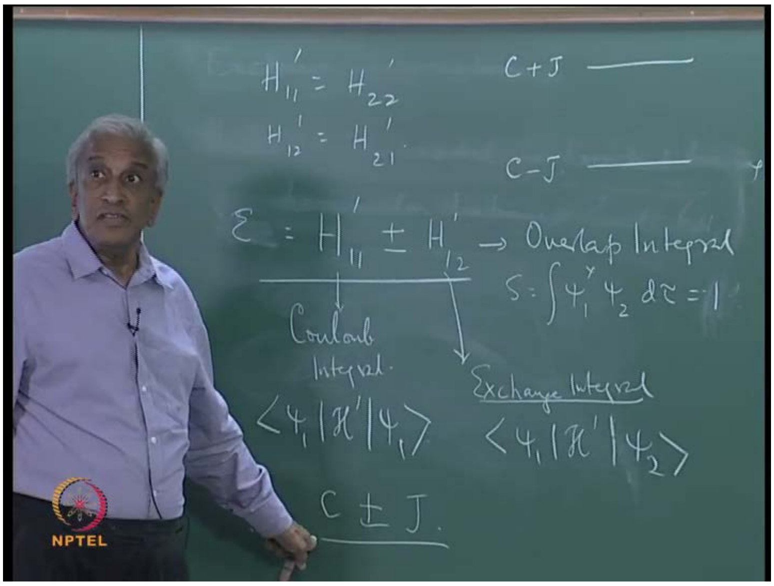

So, solving this leads to a quadratic equation. Expanding the determinant and recognising that H 2 one prime and H 2 2 prime are the same. Similarly H 1 2 prime equal to H 2 1 prime knowing this. We have a quadratic of the form which will give you have a quadratic by expanding that determinant and the roots of this quadratic are give you the energy eigenvalues.

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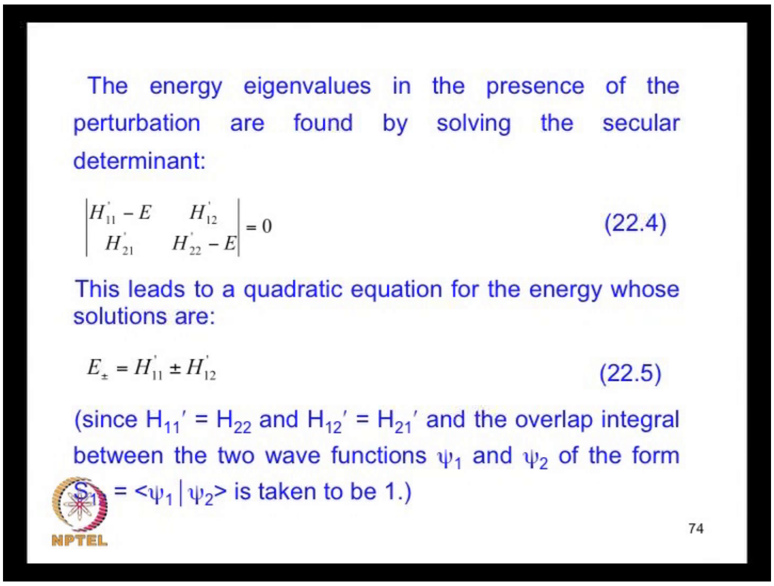

The energy eigenvalues in the presence of the perturbation are found by solving the secular determinant:

$$\begin{vmatrix} H'_{11} - E & H'_{12} \\ H'_{21} & H'_{22} - E \end{vmatrix} = 0 \qquad (22.4)$$

This leads to a quadratic equation for the energy whose solutions are:

$$E_{\pm} = H'_{11} \pm H'_{12} \qquad (22.5)$$

(since $H_{11}' = H_{22}$ and $H_{12}' = H_{21}'$ and the overlap integral between the two wave functions ψ_1 and ψ_2 of the form S = $<\psi_1 | \psi_2>$ is taken to be 1.)

So, this is going to be H 1 1 prime plus or minus H 1 2 prime now this is based on the assumption that the overlap integral of the form integral psi 1 star psi 2 the tau one if this is S equal to is taken as 1 under that assumption these are the energy eigenvalues. So, having solved the secular determinant we have got the matrix elements and what is the meaning of this H 1 1 prime is the usual integral. So, you have two possibilities this is usually known as the coulomb integral. So, this is a reform psi one H prime psi 1. So, that is the usual form of the coulomb integral, where H prime has these electrostatic terms and this is the so called exchange integral, which is of the form psi one H prime si two. This has this term has no classical analogue this means that you have this is the matrix element of the perturbing Hamiltonian, which is of a purely electrostatic character between a quantum mechanical state and this wave function corresponding to the state in which this wave function the electrons are interchanged.

So, this is therefore, it is known as the exchange integral this is a purely quantum mechanical the effect which has low classical analogue and this exchange force is of purely electrostatic origin because the perturbing Hamiltonian H prime i consist of only electrostatic attractive and repulsive terms. So, the this gives you the sum total therefore, the net energy again value there are two possibilities corresponding to the coulomb integral plus the exchange integral and the coulomb integral minus the exchange integral. So, you have the two possibilities.

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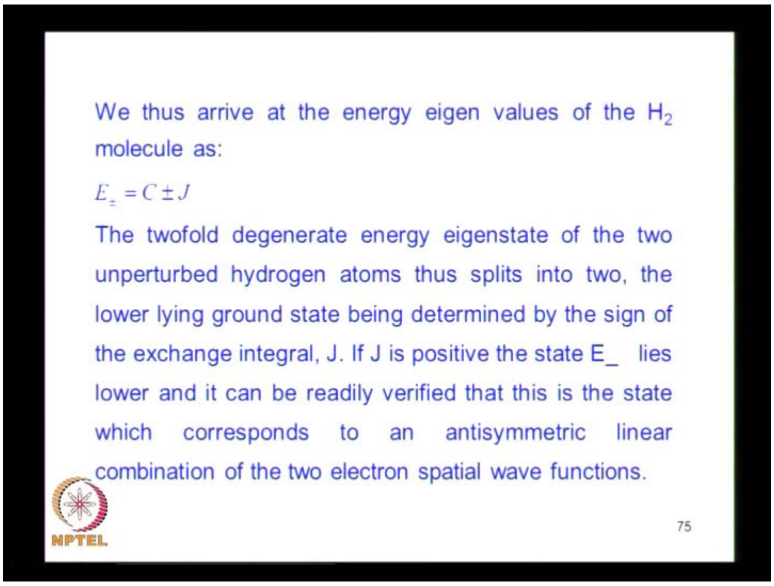

We thus arrive at the energy eigen values of the H_2 molecule as:

$$E_{\pm} = C \pm J$$

The twofold degenerate energy eigenstate of the two unperturbed hydrogen atoms thus splits into two, the lower lying ground state being determined by the sign of the exchange integral, J. If J is positive the state $E\_$ lies lower and it can be readily verified that this is the state which corresponds to an antisymmetric linear combination of the two electron spatial wave functions.

So, more often these are referred to as C plus or minus J where J is the exchange integral and C is the coulomb integral. So, now, there as a result of this they originally degenerate energy eigen states of the unperturbed hydrogen atoms this degeneracy is lifted and you have now two states 1 with the energy C plus J and C minus J according to this the state C minus J lies lower than this touched with C plus J if J is positive if J is negative then C plus J will lie lower than this C minus J term. So, which is the state which lies lower depends on the sign of the exchange integral. The exchange integral can be positive or negative and the C minus J state correspond to an anti-symmetric linear combination of the two electron special wave functions. Now this is a very interesting situation what does it means, it is this corresponds to and let us write.

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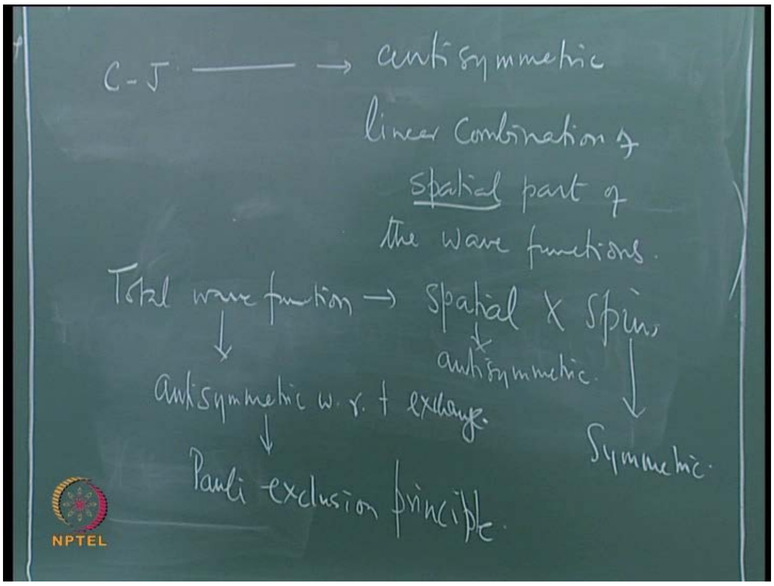

So, let us consider the situation corresponding to a positive exchange integral in greater detail if what does it mean this means that the state C minus J with energy C minus J lies lower than the state C plus J this corresponds to an anti-symmetric linear combination of this spatial part of the wave function. Now what does this mean, now the total wave function; however, consist of not only the spatial part, but also the total wave function of the system is a product of the spatial and the spin part of the wave function and according to Pauli exclusion principal. This total wave function should be anti-symmetric with respect to exchange in order to satisfy the Pauli exclusion principal, and now we know that this is a the spatial part is anti-symmetric. So, in order that the product of these two spatial and spin parts should be anti-symmetric, this means that it should be symmetric with respect to exchange of spin.

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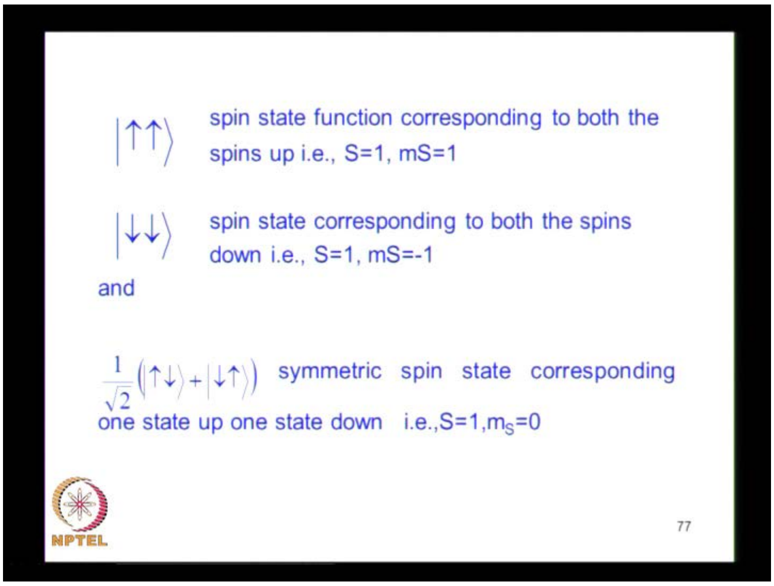

$|\uparrow\uparrow\rangle$ spin state function corresponding to both the spins up i.e., S=1, mS=1

$|\downarrow\downarrow\rangle$ spin state corresponding to both the spins down i.e., S=1, mS=-1

and

$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle\right)$ symmetric spin state corresponding one state up one state down i.e., $S=1, m_S=0$

So, let us see under what conditions the spin part of the wave function will be symmetric. So, let us look at the spins in some detail we know that the electron spin is half and therefore, you are two possibilities of the magnetic quantum number which shows the orientation of the electron spin with respect to an external magnetic field. So, if this orientation is parallel to the external feel we show it by an up arrow and if the two spins are both parallel.

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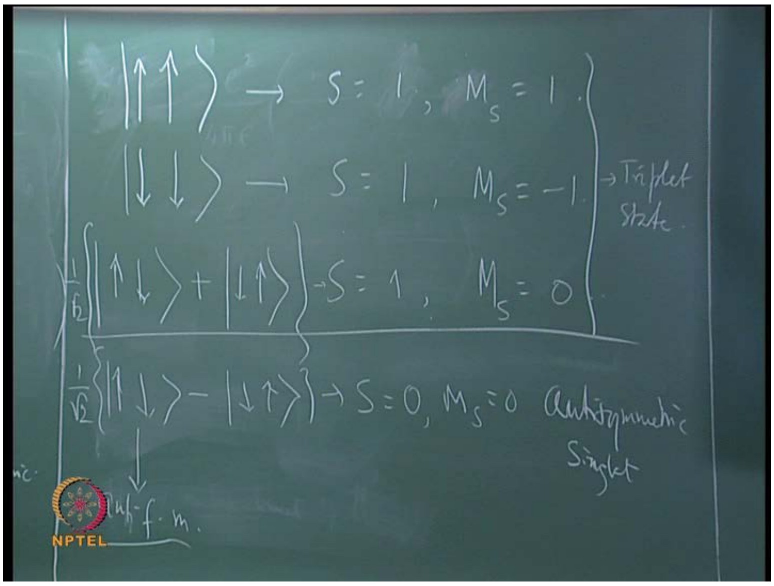

$$\left.\begin{array}{l} |\uparrow\uparrow\rangle \rightarrow S=1,\ M_S=1 \\ |\downarrow\downarrow\rangle \rightarrow S=1,\ M_S=-1 \\ \frac{1}{\sqrt{2}}\left\{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle\right\} \rightarrow S=1,\ M_S=0 \end{array}\right\} \rightarrow \text{Triplet State}$$

$$\frac{1}{\sqrt{2}}\left\{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle\right\} \rightarrow S=0,\ M_S=0 \quad \text{Antisymmetric Singlet}$$

$\downarrow$

Anti-f.m.

Then that is going to give you a spin state corresponding to the total spin which is half plus half which is 1 and that is; obviously, a state which is symmetric with respect to exchange. So, this will also have you can also have the possibility in which both this spins are anti- parallel if this is. So, this is this corresponds to M s equal to minus 1, but this still corresponds to S equal to 1. So, corresponding to S equal to 1, you have two possibilities. Now M s equal to one and M s equal to minus 1, you also have the possibility M s equal to zero and that is a state of this kind with a normalization. So, this corresponds to Ms equal to zero it is a symmetric linear combination of the states with an up arrow and down arrow and a down arrow and an up arrow.

So, all these 3 states together correspond to give rise to a spin one therefore, there are 3 states. So, this is called a triplet state. So, the one which is left out which corresponds to an anti symmetric linear combination of the spins this is anti-symmetric with respect to spin. So, this corresponds to S equal to zero Ms equal to zero and this is an anti-symmetric singlet state. So, it is these three states which are symmetric which go into this. So, this corresponds to ferromagnetic ordering. So, J greater than zero corresponds to a ferromagnetic ground state whereas, the anti-symmetric spin configuration corresponding to a singlet state with S equal to zero corresponds to a symmetric linear combination of the spatial part and that corresponds to an anti- ferromagnetic state. So, this is state C plus J is an excited state in which the two spins are anti-parallel this is in case J is greater than zero.

If J is negative on the other hand then the state C plus J with anti- parallel spins lies energetically lower than the state C minus J. So, you will have an anti - ferromagnetic ground state in this case. So, this is the basic cause of the ferromagnetic or anti-ferromagnetic ordering, and therefore, it is the sign of the exchange internal J, which determines whether a given material magnetic material will be ferromagnetic or anti ferromagnetic. This exchange integral is happens to be positive in the case of atoms like iron cobalt and nickel and that is the reason why iron cobalt and nickel are prototype ferro-magnets. Now this is the basic clue to the understanding of why the exchange interaction leads to ferromagnetic or anti-ferromagnetic ordering, but we would like to write the change Hamiltonian in a form in which the spin operators are involved. So, that the essential details of this energy level schemes are brought out by a spin Hamiltonian, involving only the spin.

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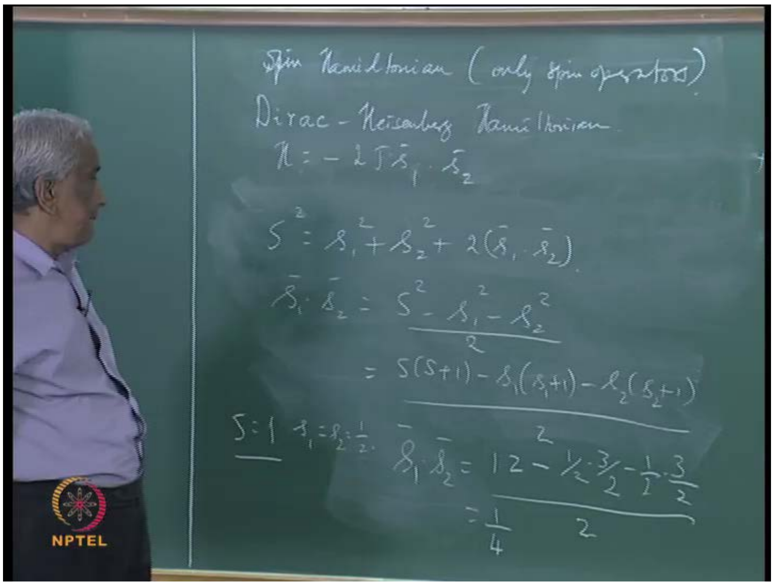

Spin Hamiltonian (only spin operators)

Dirac - Heisenberg Hamiltonian

$\mathcal{H} = -2J\bar{s}_1\cdot\bar{s}_2$

$S^2 = s_1^2 + s_2^2 + 2(\bar{s}_1\cdot\bar{s}_2)$

$\bar{s}_1\cdot\bar{s}_2 = \frac{S^2 - s_1^2 - s_2^2}{2}$

$= \frac{S(S+1) - s_1(s_1+1) - s_2(s_2+1)}{2}$

$S=1 \quad s_1=s_2=\frac{1}{2}$

$\bar{s}_1\cdot\bar{s}_2 = \frac{1\,2 - \frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot\frac{3}{2}}{2}$

$= \frac{1}{4}$

Operators involving only the spin operators, it should be we want to replace the actual Hamiltonian of the electron, two electron system by a spin Hamiltonian involving only the spin operators such that it models. The essential details of this 2 electron problem that is you have a ferromagnetic ground state which is triplet lying below the anti-ferromagnetic excited singular state by an amount equal to two J because the difference in energy is C minus J and C plus J is 2 J. So, you want to write a model Hamiltonian this was first proposed by Dirac. So, it is known as Dirac Heisenberg no it was proposed by Heisenberg. So, it is known as the Dirac Heisenberg Hamiltonian it has the form minus 2 J S 1 dot s 2. Now let us see how this leads to the same situation and how such a Hamiltonian will model our system we know that s square which is s 1 square plus s 2 square plus 2 s 1 dot.

So, we have s 1 dot s 2 is s square minus s 1 square minus s 2 square by 2 and in terms of the expectation values this is s into s plus 1 minus s 1 into s 1 plus 1 minus s 2 into s 2 plus by two. So, we have the possibility s equal to one for a triplet ground state. So, s 1 is half and s 2 is also half. So for this s 1 dot s 2 will have the value one into 2 minus half into 3 by 2 minus half into 3 by 2 by 2 and that is 3 fourth 3 4. So, this is 3 by 2. So, this will give me one fourth whereas, in the case of the singlet with total spin S equal to 0 for this.

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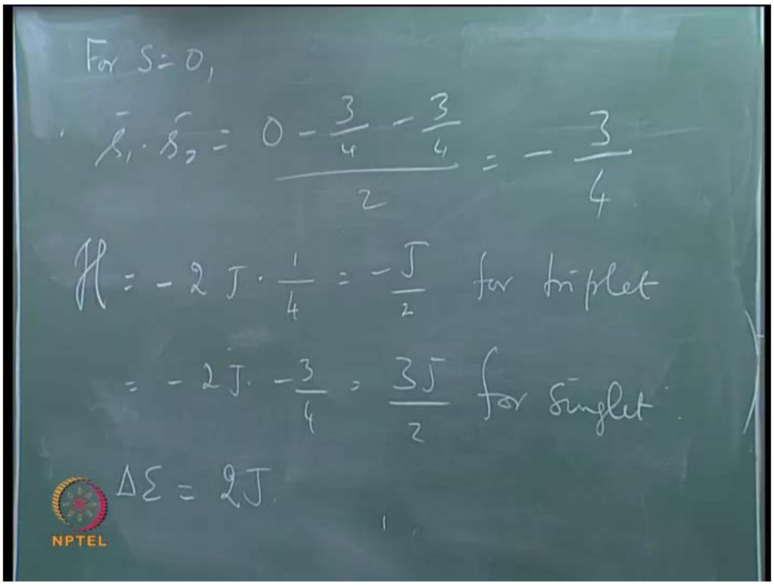

For $S = 0$,

$$\bar{s}_1 \cdot \bar{s}_2 = \frac{0 - \frac{3}{4} - \frac{3}{4}}{2} = -\frac{3}{4}$$

$$\mathcal{H} = -2J \cdot \frac{1}{4} = -\frac{J}{2} \text{ for triplet}$$

$$= -2J \cdot -\frac{3}{4} = \frac{3J}{2} \text{ for singlet}$$

$$\Delta \mathcal{E} = 2J$$

This is the energy of for S equal to 0 s 1 dot s 2 is going to be 0 minus 3 by 4 minus 3 by 4 5 2 which is minus 3 by 4. So, coming to the Heisenberg Hamiltonian, it is minus 2 J into one fourth it is minus J by 2 for triplet. And this equal to minus 2 J into minus 3 by 4 which is 3 J by 2 for this singlet, so 1 C is that the energy difference delta e between the two is 3 J by 2. So, it is plus 2 J. So, you have model the system as we wish. So, the direct Heisenberg exchange interaction Hamiltonian models our real ferromagnetic ground state. So, we use this instead of the original coulomb and exchange actual Hamiltonian terms it is this spin Hamiltonian which will be used in order to model the ground state of a real ferromagnetic material a real ferromagnetic material actually contains a large number capital n of spins. So, it is a long ranged magnetic ordering of all this n spins which gives rise to the ferro-magnet.

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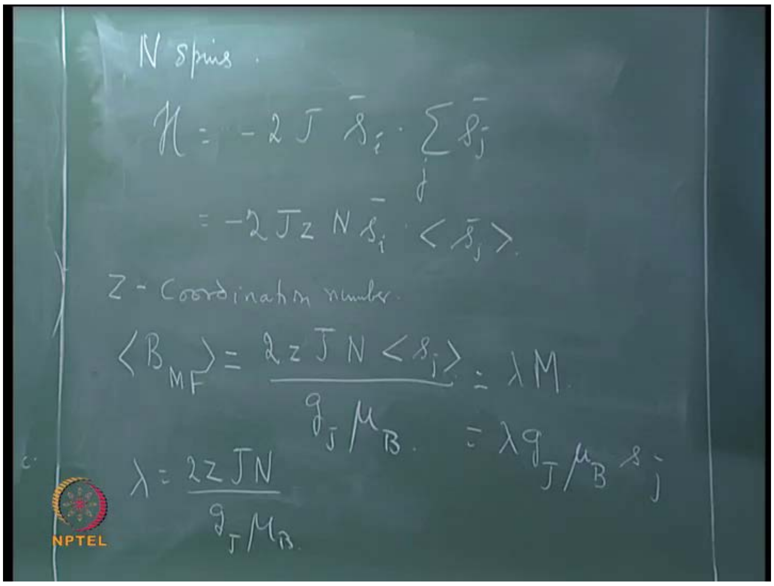

N spins.

$$\mathcal{H} = -2J\,\bar{S}_i \cdot \sum_j \bar{S}_j$$

$$= -2JzN\,\bar{S}_i \,\langle \bar{S}_j \rangle.$$

z - Coordination number.

$$\langle B_{MF} \rangle = \frac{2zJN\langle S_j \rangle}{g_J \mu_B} = \lambda M.$$

$$= \lambda g_J \mu_B S_j$$

$$\lambda = \frac{2zJN}{g_J \mu_B}$$

So, in a system of such N spins I have N a total of n spins where N is very large then we can write the total Hamiltonian as minus 2 J S 1 S 5 dot sigma S j where the summation is over j over all the N spins. So, that is the total Hamiltonian of the system. So, this can also be written as minus 2 J Z N Si dot average S J where this is the number of spins and Z is the number of near (( )). So, if we assume that the exchange coupling is non- zero only between adjacent spins. So, the summation extends over these neighbours.

So, Z is the coronation number which gives you the number of spins surrounding a given spin near neighbours and the spin is S J is the average. So, N is the total number of spins. So, this can be thought of as a mean field BM F acting on the spin and this the strength of this mean field the average is called mean field, because it is a statistical average. So, it is just two Z J N S j by g J mu B. So, if we define the magnetic field of strength given by this then this is the mean magnetic field acting on this spin. So, you have this is equal to lambda M in our original vice molecular field picture. So, this magnetization is lambda g J mu B S j.

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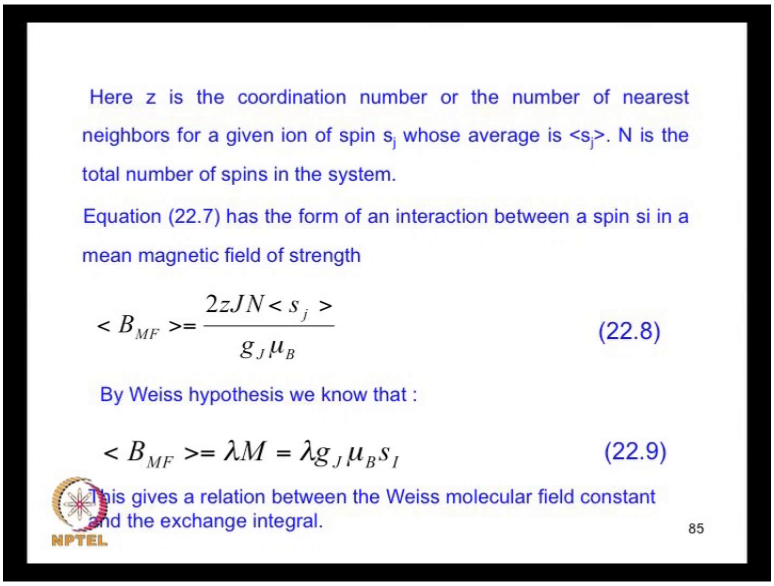

Here z is the coordination number or the number of nearest neighbors for a given ion of spin s_i whose average is $<s_j>$. N is the total number of spins in the system.

Equation (22.7) has the form of an interaction between a spin si in a mean magnetic field of strength

$$< B_{MF} >= \frac{2zJN< s_j >}{g_J \mu_B} \qquad (22.8)$$

By Weiss hypothesis we know that :

$$< B_{MF} >= \lambda M = \lambda g_J \mu_B s_I \qquad (22.9)$$

This gives a relation between the Weiss molecular field constant and the exchange integral.

Therefore we compare these two and so in terms of the exchange interaction constant J and the number of atoms or spins and the number of spin the coordination number we get an expression for the vice molecular field. So, we are in a position to relate the direct Heisenberg exchange spin Hamiltonian formalism and the mean field hypothesis enable us to obtain an expression for the relation between the vice molecular field constant lambda and the exchange integral J.

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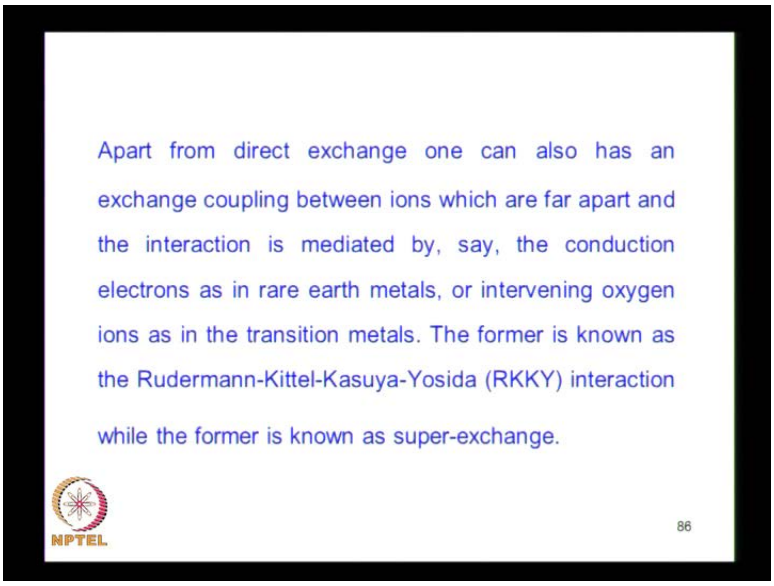

Apart from direct exchange one can also has an exchange coupling between ions which are far apart and the interaction is mediated by, say, the conduction electrons as in rare earth metals, or intervening oxygen ions as in the transition metals. The former is known as the Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction while the former is known as super-exchange.

So, we now have a microscopic understanding of the cost of the ferromagnetic or anti-ferromagnetic ordering in terms of the so called exchange interaction which is a purely quantum mechanical interaction based on the electrostatic interactions of the electrons. Now this is a direct exchange we can also have exchange interaction between ions which are far away which are not next to each other as in a homonuclear diatomic molecule, but which are very far away. But then the exchange interaction is mediated by things which are between these two far away spins what are these things these can be condition electrons this is the case in the case of rare earth metals the conduction electrons can mediate.

In other word the spin of one ion can interact with an electron with a conduction electron which is free to wander around and that conduction electron in turn interacts with the other ion. So, there is effect in effect in extreme coupling between the two ion mediated by the conduction electrons. This is what happens in the case of the rare earth metal in the case of transition metals you have metal compounds containing say oxygen atoms transition metal oxides like manganese oxide. For example, you have the mediation between the two ions the exchange interaction is caused by intervening oxygen ions. So, one ion the spin interacts with the neighbouring oxygen ions oxygen spin and this oxygen spin in turn interacts with the other ion. So, you have an exchange interaction between the two transition metal ions mediated by the intervening oxygen spins of the oxygen ions.

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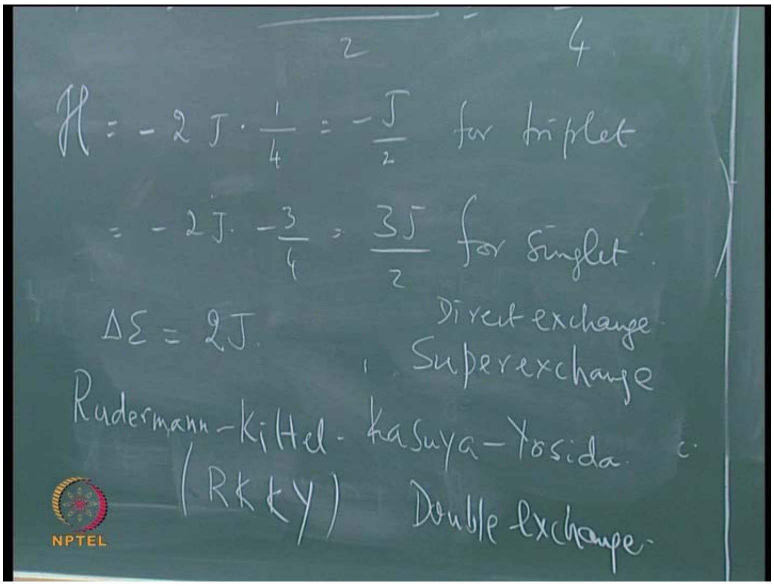

$$\mathcal{H} = -2J \cdot \frac{1}{4} = -\frac{J}{2} \text{ for triplet}$$

$$= -2J \cdot -\frac{3}{4} = \frac{3J}{2} \text{ for singlet}$$

$$\Delta E = 2J$$

Direct exchange

Superexchange

Rudermann-Kittel-Kasuya-Yosida (RKKY)

Double exchange

So, this is known as the super exchange the conduction electron mediated exchange interaction was first proposed by these people Rudermann, Kiltel, Kasuya and Yosida. So, this is known as RKKY interaction. So, the conduction electron mediated exchange interaction is known as the RKKY interaction and that is responsible for the ordering of rare earth metals. Whereas, the exchange mediated by oxygen ions in transition metal oxide is known as the super exchange. So, we have direct exchange super exchange and then RKKY interaction. So, these are the different kinds of exchange interactions.

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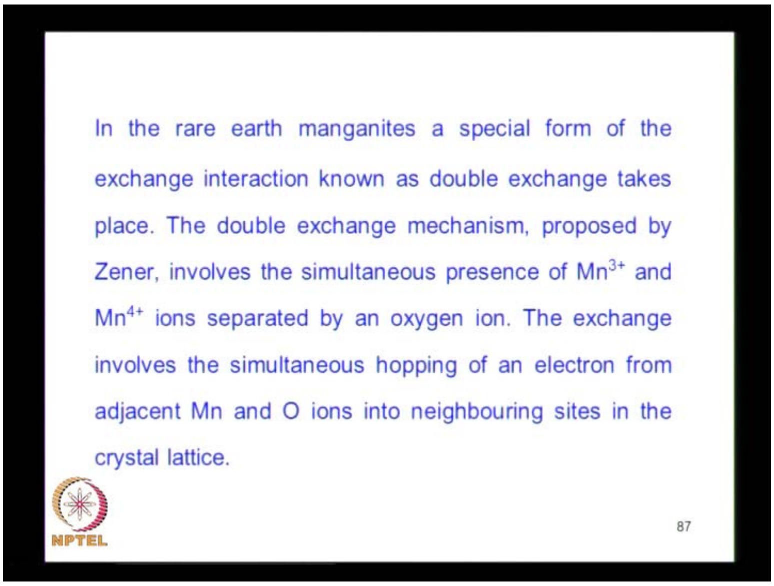

In the rare earth manganites a special form of the exchange interaction known as double exchange takes place. The double exchange mechanism, proposed by Zener, involves the simultaneous presence of Mn^{3+} and Mn^{4+} ions separated by an oxygen ion. The exchange involves the simultaneous hopping of an electron from adjacent Mn and O ions into neighbouring sites in the crystal lattice.

There is an another interesting family known as the rare earth manganites in which there is a special form of exchange interaction known as double exchange in the manganites there are manganese ions. So, you have a manganese two plus and a manganese 3 plus ions separated by an oxygen ion. So, the exchange involves the simultaneous hoping of an electron from adjacent manganese and oxygen ions into neighbouring sides in the crystal lattice. So, that an Mn 2 plus becomes an Mn 3 plus and the MN 3 plus becomes an Mn 2 plus. So, there is a double exchange mechanism there is a simultaneous hoping of an electron. So, this is known as the double exchange mechanism. So, these are the various forms of exchange interactions.

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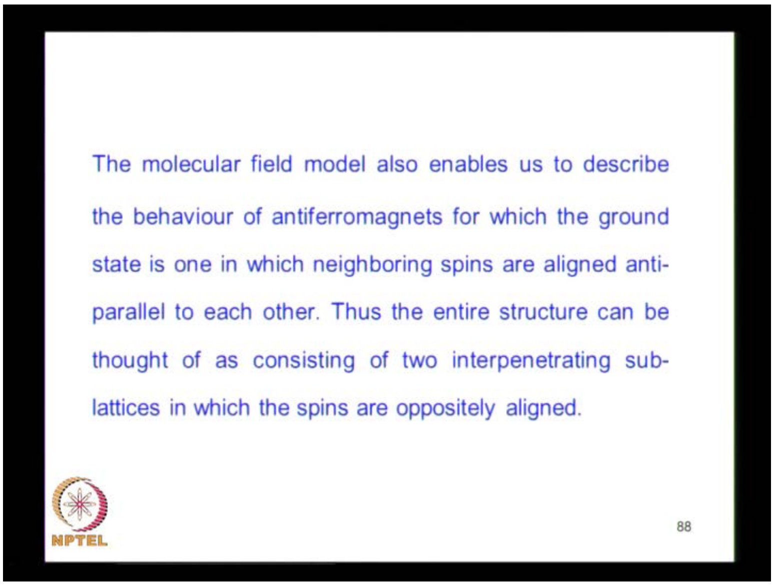

The molecular field model also enables us to describe the behaviour of antiferromagnets for which the ground state is one in which neighboring spins are aligned anti-parallel to each other. Thus the entire structure can be thought of as consisting of two interpenetrating sub-lattices in which the spins are oppositely aligned.

Now, the molecular field model can also be used to describe the behaviour of anti ferromagnets for which as we have already seen the ground state is that of a anti parallel spins which are aligned anti parallel to each other. So, the entire structure can be thought of as consisting of two inter penetrating sub lattices in which the spins are oppositely aligned. So, you can have a picture in which there are inter penetrating sub lattices. So, you have a two sub lattice model for example, of an anti- ferromagnetic solid. So, the molecular field hypothesis enables us to write the interactions in the presence of an applied magnetic field as follows.

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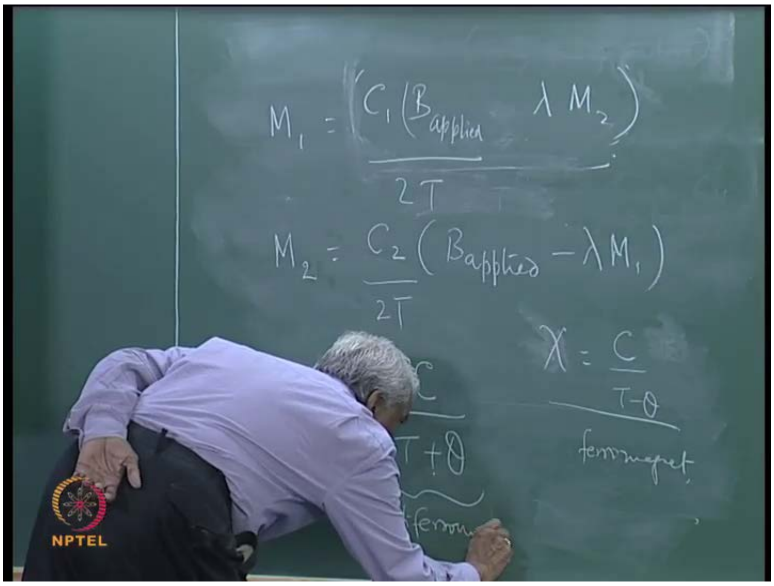

So, you have the possibility to write the magnetization in the first sub lattice is given by the curie constant times B minus lambda M right lambda M 2 this is the applied field. So, this is the total this is the C 1 B by 2 T the factor two comes because you have an half the lattice is divided into two. There are two interpenetrating sub lattices, the curie constant therefore, gets to the form C one by 2 number. This will be the local field similarly we can write a similar equation for the other sub lattice where T is the temperature. So, solving these two equation simultaneously we will get the total curie constant and the magnetization of the two sub lattices solving these two together.

We find that for an anti ferromagnet which is in the paramagnetic phase that is above the curie temperature the magnetic susceptibility follows a curie vice behaviour, but with the magnetic the total magnetization is of the form a curie vice behaviour, but with a positive sign for it is C by T plus theta we may recall that for a ferromagnet. It was the form C minus theta this is the we can write the susceptibility in the paramagnetic state. So, this is the ferromagnet this is the behaviour of the susceptibility for an anti ferromagnet.

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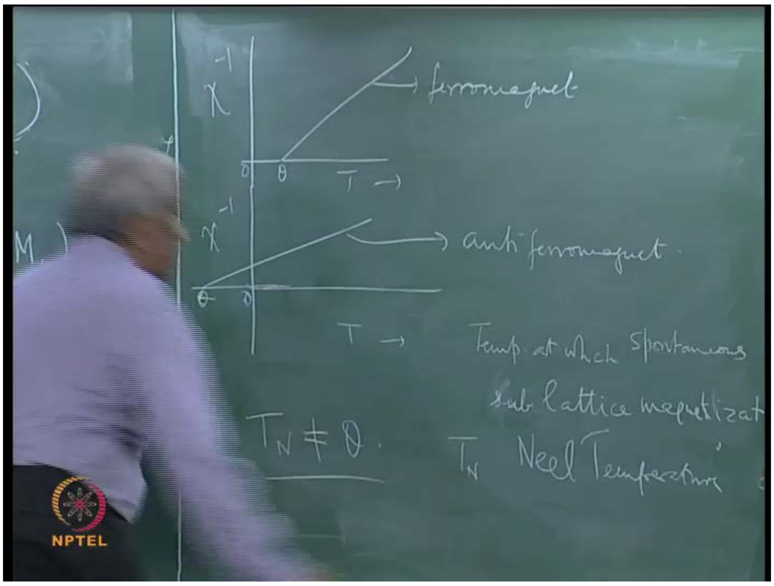

So, if we plot the susceptibility temperature dependence of the inverse susceptibility as before then we get we saw that already that (( )) verses T is something like this for a ferromagnet with this as the paramagnetic curie temperature whereas, for an anti ferromagnet. So, this zero. So, we have a negative intercept this is theta. So, this is the behaviour of an anti ferromagnet above the ordering or curie temperature or the curie wise temperature theta. So, we can easily distinguish between the behaviour of a ferromagnetic material and an anti-ferromagnetic material even by measuring the paramagnetic susceptibility above the curie wise temperature. So, you will have a negative intercept in the case of an anti ferromagnet whereas, it will have a positive intercept for a ferromagnet.

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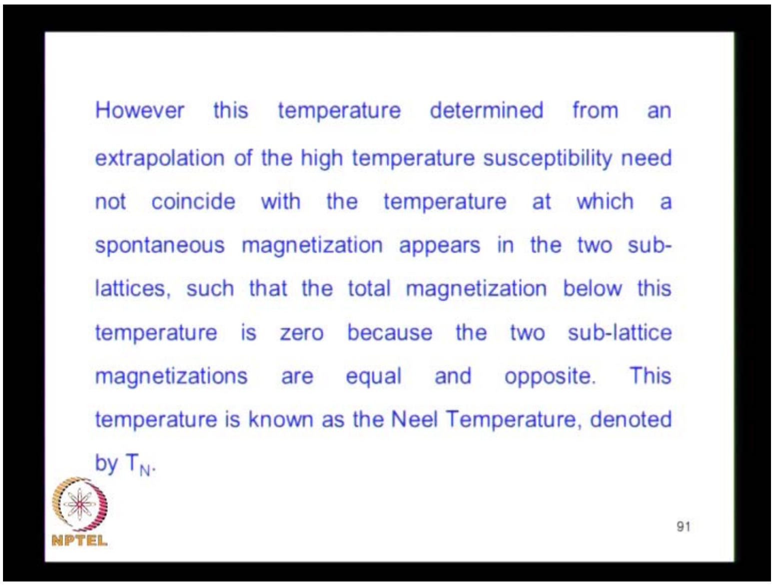

However this temperature determined from an extrapolation of the high temperature susceptibility need not coincide with the temperature at which a spontaneous magnetization appears in the two sub-lattices, such that the total magnetization below this temperature is zero because the two sub-lattice magnetizations are equal and opposite. This temperature is known as the Neel Temperature, denoted by T_N.

The temperature determined from an extrapolation of the high temperature susceptibility that is this theta need not coincide with the temperature at which a spontaneous magnetization appears in the two sub lattices. See, we must understand that there is this is the curie wise temperature which is measured by measuring the inverse susceptibility and plotting. It as a function of temperature in the paramagnetic state, but the actual ordering temperature the critical temperature the magnetic ordering temperature is the one in which a spontaneous magnetization appears in the two sub lattices if there is a spontaneous magnetization and since in an anti ferromagnet the spins are aligned anti parallel to each other the two sub lattices have equal, but opposite signs for this spontaneous magnetization.

Therefore, the total magnetization is zero even though the individual sub lattice magnetization are non- zero because these two sub lattice magnetization are equal in magnitude, but opposite in direction. So, the temperature at which such a thing happens the temperature at which spontaneous sub lattice magnetization appears is known as the

Neel temperature TN in general TN is not equal to theta even in magnitude. So, the Neel temperature is the actual temperature of the ordering, but then how do you detect anti ferromagnetic ordering if you measure the total magnetization it is zero as in the paramagnetic state. So, you have to really look at the sub lattice ordering there is no way in which you can measure the magnetization in the sub lattice.

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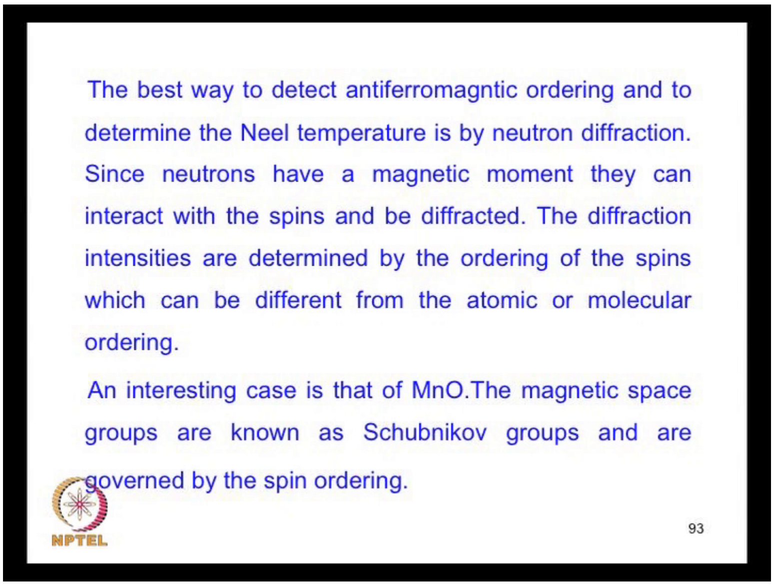

The best way to detect antiferromagntic ordering and to determine the Neel temperature is by neutron diffraction. Since neutrons have a magnetic moment they can interact with the spins and be diffracted. The diffraction intensities are determined by the ordering of the spins which can be different from the atomic or molecular ordering.

An interesting case is that of MnO.The magnetic space groups are known as Schubnikov groups and are governed by the spin ordering.

So, in order to determine the Neel temperature and actually observe the magnetic ordering in the two sub lattices in an anti- ferromagnet the best way is to employ neutron diffraction neutrons have a magnetic moment. So, they can interact with the spins and be diffracted. So, the diffraction intensities are determined by the ordering of the spins which can be different from the atomic or molecular ordering. So, this is what we will see for example, in an magnetically anti ferromagnetically ordered solid like manganese oxide. We will look at this in detail in the next lecture.