Advanced Quantum Mechanics with Applications
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Lecture – 12
Magnetic Hamiltonian, Heisenberg Model

Let us now discuss; how one gets a Magnetic Hamiltonian involving only spins. We are particularly talking about Ising kind of Hamiltonian or Heisenberg kind of Hamiltonians. Mainly, we would be talking about Ising Hamiltonians where the spin can only have either pointing up or down these are the two possible orientations. And let us see that how we can derive a Hamiltonian which we have introduced or rather we have talked about when we spoke on magnetism during our lectures.

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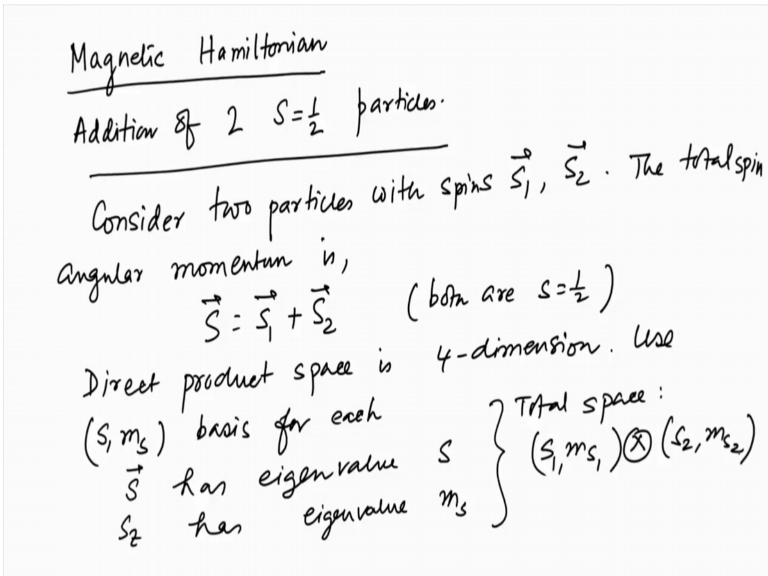

So, we want to study magnetic Hamiltonian and a derivation of a magnetic Hamiltonian would require that we know the addition of spins or so, say addition of 2 spins 2 and these are spin half particles. So, we have 2 spin half particles and we would see that how one actually add the spin vectors. So, let us consider two particles with spin vectors S 1 and S 2, the total angular momentum I mean what I mean by angular momentum is that the total spin angular momentum is S equal to S 1 plus S 2. Where S 1 and S 2’s are the spin vectors for the two particles that we are considering so, just to remind you that both are spin half.

Now, the direct product space is that consists of it is of 4 dimensions. So, that direct product space is 4 dimensional and we can use the basis use S m s basis for each. So, what I mean by that is that the eigenvalue for the spin operator S is has eigenvalue s and s z has eigenvalue m s. So, we can form the basis of each of the particles by this S m s and the total space will be product of such to such S m s's that is s 1. So, total product total space is S 1 m s 1 and S 2 m s 2.

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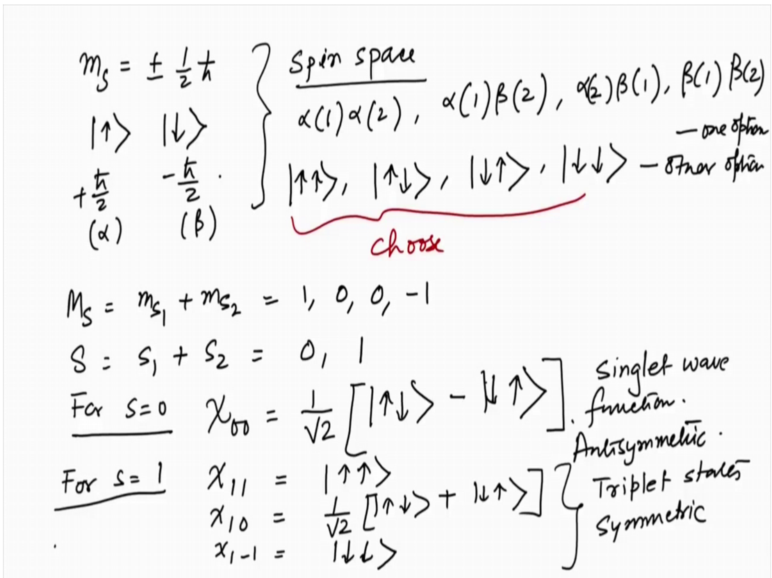

And let the since we have for each one of them so m s is equal to plus minus half h cross; so, let us represent the states by up and down. So, each of these half h will correspond to say a up and this minus half will correspond to minus half h cross. So, this h cross over 2 and this is minus h cross over 2 and hence we will have we can write it in two ways. So, the space the spin space or the direct product space is either you call it alpha 1. So, maybe this is called as a alpha and this is called as a beta or so it is alpha 1 alpha 2 which means both are in up spin states, alpha 1 beta 2 means one of them in up spin the other in down spin state.

And alpha 2 beta 1 the first one is in the down and the second one is in up or both of them are in the down. And this is one option where as the other option is that we can write it as up up as the states, up down and down up and down down. So, this is other option and we can simply choose one of them, but let us choose this option in order to write the wave function for the or and I mean to discuss this problem of 2 spins.

So, what is the total value of M S which is m s 1 plus m s 2, m s 2 which can take value 1, 0, 0, minus 1; 1 when they both add up half plus half and this is when half minus half this is minus half half and this is minus half minus half. And the total spin quantum number S which is equal to s 1 plus s 2, which can take value 0 and 1 ok. So, for s equal to 0 for s equal to 0; we have there just 1 eigen function and that eigen function let us write it with a form which is chi 0 0 which is equal to 1 over root 2.

And I have a up down minus a down up. So, this is; the this is called as a singlet wave function and this is antisymmetric, what I mean by antisymmetric is the following; that you have two particles. So, the first one is in upstate the second one is in downstate, here the second one the first one is in downstate and the second was in is in upstate. And now if you interchange up to down one gets a negative sign. So, this is that is why it is called as a antisymmetric and for s equal to 1 we would need so for s equal to 1 we will have three combination because, we will have to take care of chi 1 1 which will be simply a up up state chi 1 0 which will simply be a combination of up down plus a down up and a chi 1 minus 1 which is equal to a down down state.

Now, all these are called as triplet and triplet states because they are three in number and one can easily check that they are symmetric because, if the first particle is written swapped with the second particle the wave function remains the same. So, these are the states or the wave functions for 2 particles both spin half and for a system consisting of or comprising of 2 spin half particles and all possible combinations have been taken. We get 4 states and those 4 states are one singlet and three triplet states, the singlet state is a antisymmetric with respect to the change in the position of the particle and the triplet states are symmetric with respect to the change in the position of the particle.

So, these are the states, but what about the eigenvalues, because in order to solve a full quantum mechanical problem we both we need the both the information on the eigenvalues and the eigen functions.

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$|\uparrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ — basis of a 2 particle ($s=\frac{1}{2}$) system

They are eigenstates of $\vec{S}_1^{\,2}, \vec{S}_2^{\,2}, S_{1z}, S_{2z}$.

Total spin, $S = 0, 1$

$$S_z|\uparrow\uparrow\rangle = (S_{z} + S_{2z})|\uparrow\uparrow\rangle = \hbar|\uparrow\uparrow\rangle \;;\; S_z|\uparrow\downarrow\rangle = 0$$

$$S_z|\downarrow\uparrow\rangle = 0, \quad S_z|\downarrow\downarrow\rangle = -\hbar|\downarrow\downarrow\rangle$$

Furthermore, $\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)^2 = \vec{S}_1^{\,2} + \vec{S}_2^{\,2} + 2\vec{S}_1\cdot\vec{S}_2$

$$\vec{S}^2|\uparrow\uparrow\rangle = \hbar^2\tfrac{1}{2}(\tfrac{1}{2}+1) + \hbar^2\tfrac{1}{2}(\tfrac{1}{2}+1) + 2\vec{S}_1\cdot\vec{S}_2$$

$$\vec{S}_1\cdot\vec{S}_2 = S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z \qquad S_+ = S_x + iS_y, \quad S_- = S_x - iS_y$$

$$= \tfrac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+) + S_1^z S_2^z$$

So, let us see that say all these 3 states so, now, will talk about the eigenvalues these states are up up, up down, down up and down down. And so, this forms the basis of the problem of a 2 particle problem, 2 particle spin half system. So, they are eigen states of S 1 square, S 2 square, S 1 z and S 2 z. So, the total spin S can be 0 or 1 ok.

So, now we can see the how these total spin operators act on those each of the states. So, the total spin operator which is S z which is equal to S 1 z plus S 2 z that acting this state acting on or let us write it here as well. So, S z acting on the up up, state up up this will give me S 1 z will only act on the first spin on the left and S 2 z will act on the spin on the right. So, this will give me h cross by 2 for each one them and I will get a h cross by 2 and a up up.

So, as we have said that these are eigen states of these operators so, I get an eigenvalue equation which is S z acting on a up up state gives me h cross by 2 as a eigenvalue and returns me the up up state is well. Similarly for S z acting on up down would give me 0 because S 1 z will give me a plus h cross by 2 and S z 2 will give me a minus h cross by 2 and similarly, we will also have S z acting on the down up state should also give me 0. And S z now acting on the down down state will give me a minus h cross sorry this is a minus h cross by 2 for each. So, this should be simply h cross.

So, this is for each one of them there is an h cross by 2. So, there is there are 2 h cross by 2 which make as h cross. So, S z on down down will give me a minus h cross and so on.

So, these are the eigenvalues of these S z operator and what about so further more we have a S square which is equal to S 1 square which is S 1 plus S 2 whole square which is equal to S 1 square plus S 2 square plus twice of S 1 dot S 2 S 1 and S 2 will commute with each other because they are they pertain to different particles.

So, S 1 square will be h cross so, it is half into half plus 1, half into half plus 1 this acting on so, S square acting on any of these states. So, say we will talk about up up say for example. So, this is equal to half into half plus 1 sorry if S into S plus 1. So, that is this and then again for the S 2 square this will be half into half plus 1 now we of course, do not know the what is 2 S 1 plus S 2. So, we will leave it for the moment and let us see that what we can do for the S 1 dot S 2.

So, S 1 dot S 2 if you see it is equal to S 1 x S 2 x plus S 1 y S 2 y S 2 y plus S 1 z S 2 z. Now, if you introduce this ladder operators for the spins so, S plus can be written as S x plus i S y and S minus can be written as S x minus i S y. Now this will give me S 1; plus S 2 minus plus S 1 minus S 2 plus and then there will be a factor of half there and plus S 1 z S 2 z so, this is S 1 dot S 2.

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$$\vec{S}^2|\uparrow\uparrow\rangle = \left[\frac{3}{4}\hbar^2 + \frac{3}{4}\hbar^2 + 2\left(\frac{\hbar}{2}\right)\right]|\uparrow\uparrow\rangle$$
$$= 2\hbar^2|\uparrow\uparrow\rangle$$
$$\vec{S}^2|\downarrow\downarrow\rangle = 2\hbar^2|\downarrow\downarrow\rangle$$

States $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ have total spin $S=1$, $m_s=\pm\hbar$

$m_s=0$ state is obtained by the application of S^- on $|\uparrow\uparrow\rangle$ (or S^+ on $|\downarrow\downarrow\rangle$)

$$S^-|\uparrow\uparrow\rangle = (S_1^- + S_2^-)|\uparrow\uparrow\rangle = \hbar\left[|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right]$$
$$\frac{1}{\hbar}S_-|\uparrow\uparrow\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] \Rightarrow$$ Correspond to $S_z = 0$.

$\Rightarrow$ Triplet states

And hence what we can do is that we can see that S square acting on a up up which we have already saw that the first term gives three-fourth h cross square second term gives three-fourth h cross square as well.

Now, we have a 2 S 1 dot S 2, now for the up up state this will raise the spin and hence it will be 0 because up is the maximally aligned state and though S 2 minus can give you a non zero contribution, but S 1 plus will give 0. And similarly S 2 plus will give 0 and that is why these 2 terms do not contribute and that simplifies the problem and then we are left with S 1 z S 2 z for which we know the operation. So, that is why we have done this and this is 2 into h cross by 2 and this whole thing and this whole thing multiplied or rather acted upon by this.

So, it is eigenvalue equation and this is if you simplify it becomes equal to 2 h cross square up up and so on. And similarly for the down down is well one gets the same answer by doing the same technique one gets this as so on these acting on the down down state will give us a 2 h cross square and a down down. And so, they have so, these states up up and down down have total spin S equal to 1 and m s equal to plus minus h cross ok.

But of course, S equal to 1 should have three states; which are equal to m s plus minus h and 0. So, the third state so, m s equal plus minus h is there. So, m s equal to 0 state is obtained by a particular operation. So, by the application of S minus on up up state let us see how one gets it or you can also consider or S plus on the down down states. So, S plus S minus on the up up state gives me S 1 minus plus a S 2 minus on the up up state which gives me so, S 1 minus will lower this spin. And now this is something that you should have done in quantum mechanics, this gives me an eigenvalue which is these are not eigen states of up up.

But it will operate on this and give me this S 1 will give me a h cross and will give me up down, sorry it will be a down up the first one will lower. So, it is a down up plus and up down S 2 will lower the other one with an eigenvalue which is given by h cross.

And so, 1 over h cross S minus; up up is nothing, but 1 by root 2 which comes as a normalization factor up down plus down up does not matter we have written down the second term ahead of the first term. And this will correspond to S z equal to 0 so, these three will be called as the triplet states. And so, the singlet states are of course, the which corresponds to so, these are the triplet states.

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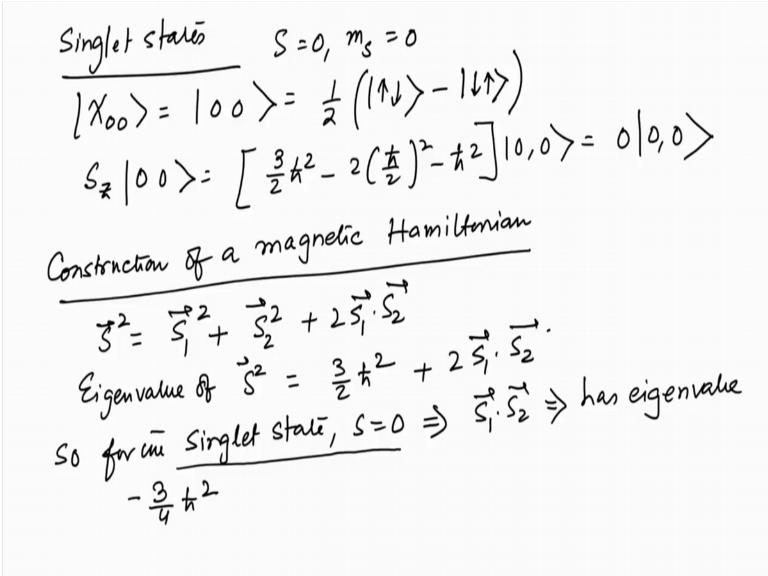

So, the two that is coming over here with spin S equal to 1 and m s equal to one which is here and the other one comes from here so, these are the three states. And now we will just look at the singlet state. So, which corresponds to S equal to 0 m s equal to 0, let us just call it as we can call it as chi 0 0 or we can also use a notation which is like 0 0, which is equal to a half up down minus down up.

So, why is it a singlet state? So, S z acting on this 0 0 will give me a 3 by 2. So, it is S 1 z plus S 2 z which will act on this it will be a 3 by 2 h cross square minus 2 into h cross by 2 square minus h cross square acting on 0 0 and it will give me a 0 0 0. So, which means that m s value of this is equal to 0 and this has S equal to 0. So, we have found out all the four eigen states of this of these 2 particle problem. So, let us now; look at the spin Hamiltonian consisting of these, if you want to construct a Hamiltonian only consisting of these two spins which is like a as I said as like a Ising Hamiltonian or a Heisenberg Hamiltonian if S has a full rotational symmetry.

So, let us just discuss the construction of a magnetic Hamiltonian. So, we have S square which is equal to S 1 square plus S 2 square plus a 2 S 1 dot S 2. Now the eigenvalue of eigenvalue of S square is equal to 3 by 2 h cross square as we have discussed that 3 by 3 coming comes from 2 terms of 3 by 4 h cross square each of S 1 and S 2 and plus a 2 S 1 dot S 2. So, for the singlet state that is S equal to 0, we will have to put S equal to 0 the S 1 S 1 dot S 2 has an eigenvalue, which is equal to minus half minus 3 4th h cross square.

Because this is equal to 0, if you put the right hand side equal to 0 the S 1 dot S 2 will have an eigenvalue which is half of a minus of half of 3 by 2 h cross square which is minus 3 by 4 h cross square.

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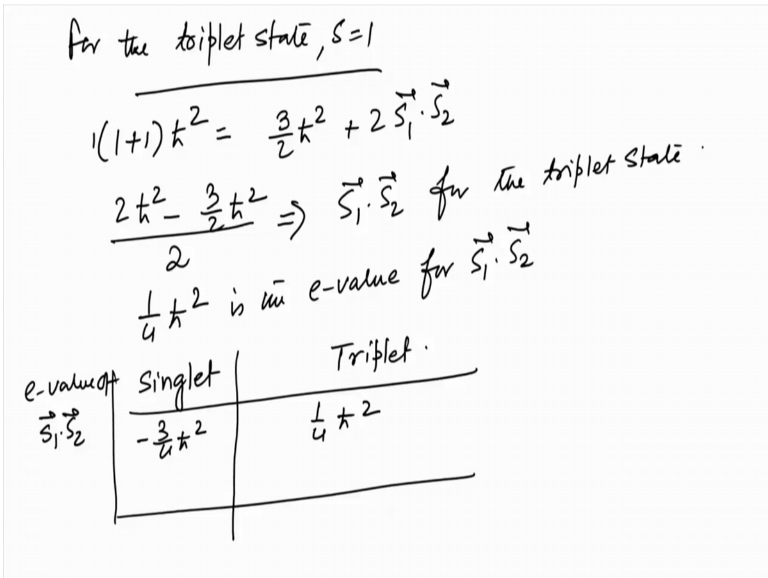

Whereas for the triplet state which corresponds to S equal to1. So, that will have 1 into 1 plus 1 h cross square for the left hand side, which is equal to a 3 by 2 h cross square and plus twice of S 1 dot S 2 so, this is equal to 2. So, 2 h cross square minus 3 half h cross square divided by 2 is the eigenvalue for S 1 dot S 2 for the triplet state.

So, this is equal to 2 minus 3 half is just half. So, this is equal to one-fourth h cross square. So, one-fourth h cross square is the eigenvalue in short e value I am writing for the operator S 1 dot S 2 in the for a 2 particle problem. So, let us just summarize this quick result. So, for singlet states S 1 dot S 2 so this is singlet and triplet. So, this singlet one has minus 3 by 4 h cross square and this is one-fourth h cross square. So, this is the eigenvalue of S 1 dot S 2.

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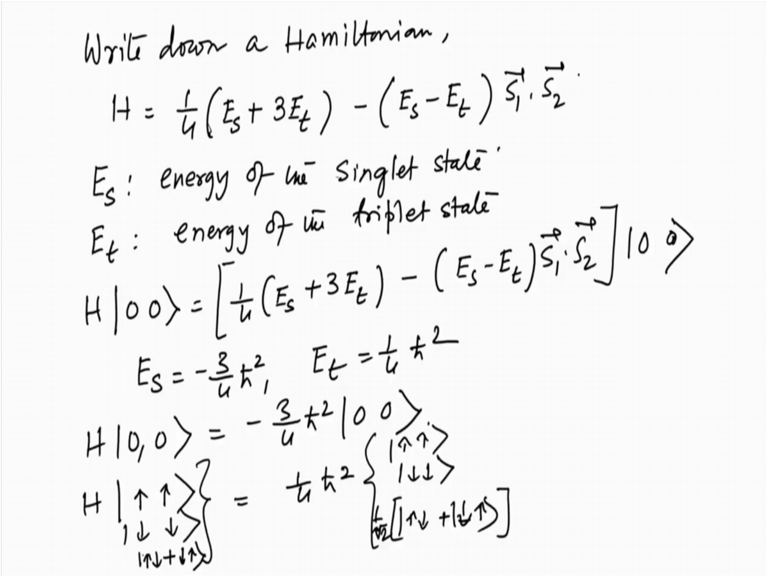

Now, if we write down a Hamiltonian, which is H equal to one-fourth E s plus 3 E t I will tell you what these are E s minus E t S 1 dot S 2. We have written it in a particular way a this term where E s is the energy of the singlet state and E t is the energy of the triplet state.

And why have we written it in this fashion is that H acting on the singlet state which is 0 0 will be simply equal to this one-fourth E s plus 3 E t and E s minus E t S 1 dot S 2 acting on 0 0. We can skip the comma in between so that is the singlet state. So, with E s equal to minus 3 by 4 h cross square and E t equal to one-fourth h cross square one can simply check that H of 0 will give me a minus 3 by 4 h cross square 0 0.

And similarly H acting on either of these; up up states or down down states or up down plus down up states all those multitude of you know down down or up down plus down up, up down plus down up state with a normalization will give me a 1 by 4 h cross square and these states that we have written such as up up, down down, up down plus down up.

So, that says that we have arrived at a Hamiltonian which is which gives us for a 2 particle problem which gives us the correct energy eigenvalues for 2 spin half particles for a system of 2 spin half particles and this is that Hamiltonian.

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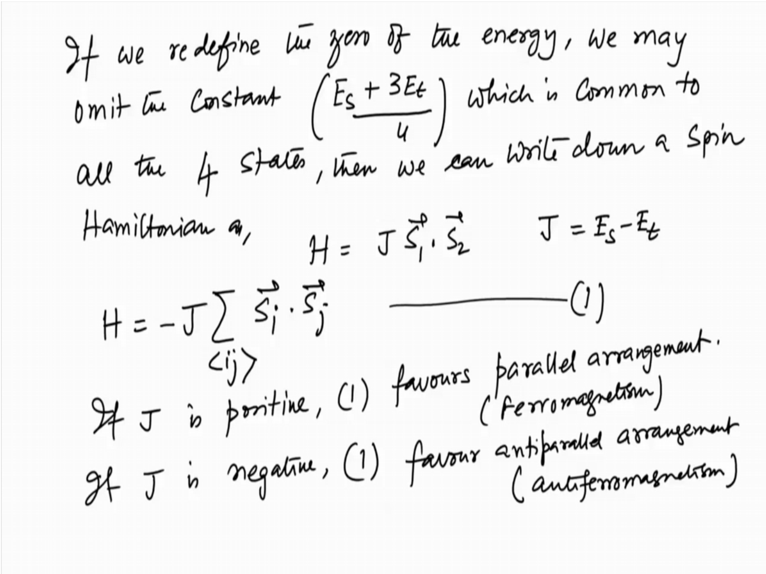

Now you can see that if you if we redefine the zero of the energy we may omit the constant E s plus 3 E t by 4 which is common to all the states all the all the 4 states. Then we can write down a Spin Hamiltonian, Spin Hamiltonian as H equal to J into S 1 dot S 2, where J is nothing, but the difference between the singlet and the triplet energies here of course, we have the singlet energy to be a lower which is equal to minus 3 by 4 h cross square. And E t being a 1 4th h cross square so, J will be negative.

Now if we say that such Hamiltonians can be written for n particles with a pair wise interaction between the particles, then we can write a generic Hamiltonian for a magnetic system or spin half system. We can extend it to a spin having any values it should be then it is a J and then there is a S i dot a S j it is i and j. It is between the neighboring sides and this is Heisenberg Hamiltonian if S has a full rotational symmetry.

And it is just the Ising Hamiltonian if S is taken as plus minus half, but; however, it gives magnetic properties of the magnetic system such as antiferromagnet or ferromagnet. And of course, its if J is positive now we are not considering, restricting ourselves to only 2 particles were we know that J is negative, but we also consider go ahead and consider J to be positive is well.

So, if J is positive in this particular model in this Hamiltonian given by 1, 1 favours we can write it with a minus sign putting a minus sign from outside. Then this favours parallel arrangement of spins and which are essential for ferromagnetism. And if J is negative then 1 favours antiparallel arrangement. And it is antiferromagnetism is, we have seen these phenomena from a purely electronic model which is Harvard model, but; however, we have also got an exposed to this kind of spin only models which are there.

So, if J is positive then the energy is lowered if the S i dot S j that is the S i and S j they point the spin vectors point in the same direction. Which are in a sense we talk about ferromagnetism whereas, if J is negative then; that means, that the whole energy would be negative if S i and S j are antiparallely aligned which are the features of antiferromagnetism.

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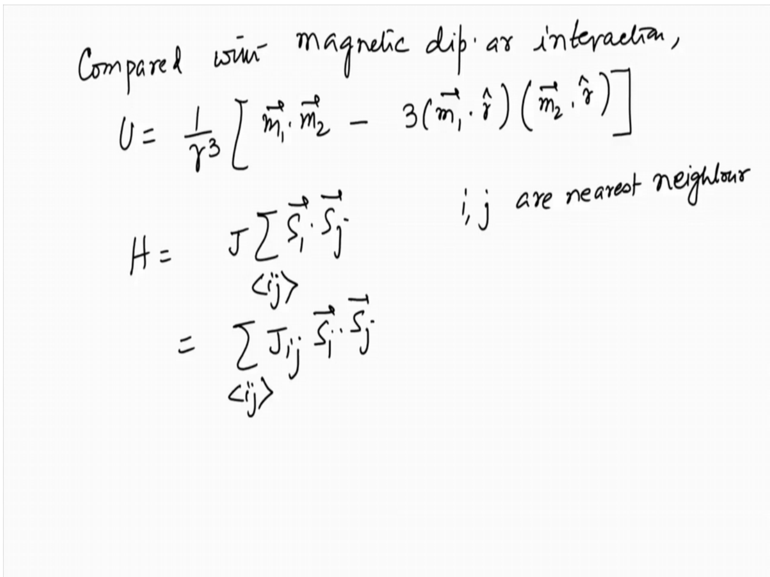

And so, this can be actually compared with the magnetic dipolar interaction like this which is 1 over r cube and it is a m 1 dot m 2 so, these are the two magnetic moments. And these are related this you are familiar in the context of classical electromagnetic theory. And the relative distance where the relative distance between m 1 and m 2 are involved, but here we have a purely spin Hamiltonian which neglects all special symmetries. Now this is H written as J S i dot S j has there are a large number of approximation that are going on.

Namely i j are nearest neighbors one does not have to be one can include; or longer than nearest neighbor that is next to next nearest neighbor interactions is well. And we can also write this inside the J to be inside and it does not have to be constant and it can depend from a one bond to another. And so, these are these are possible Hamiltonians and they have all been explored in the context of spin systems.