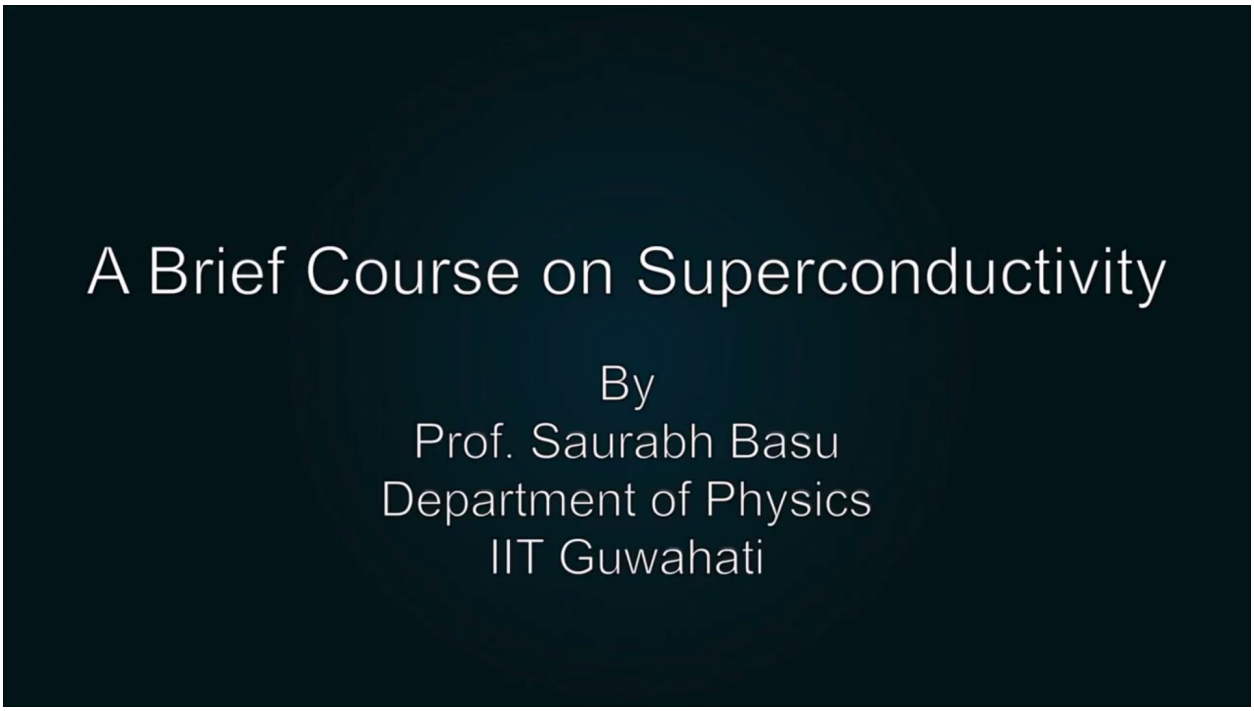
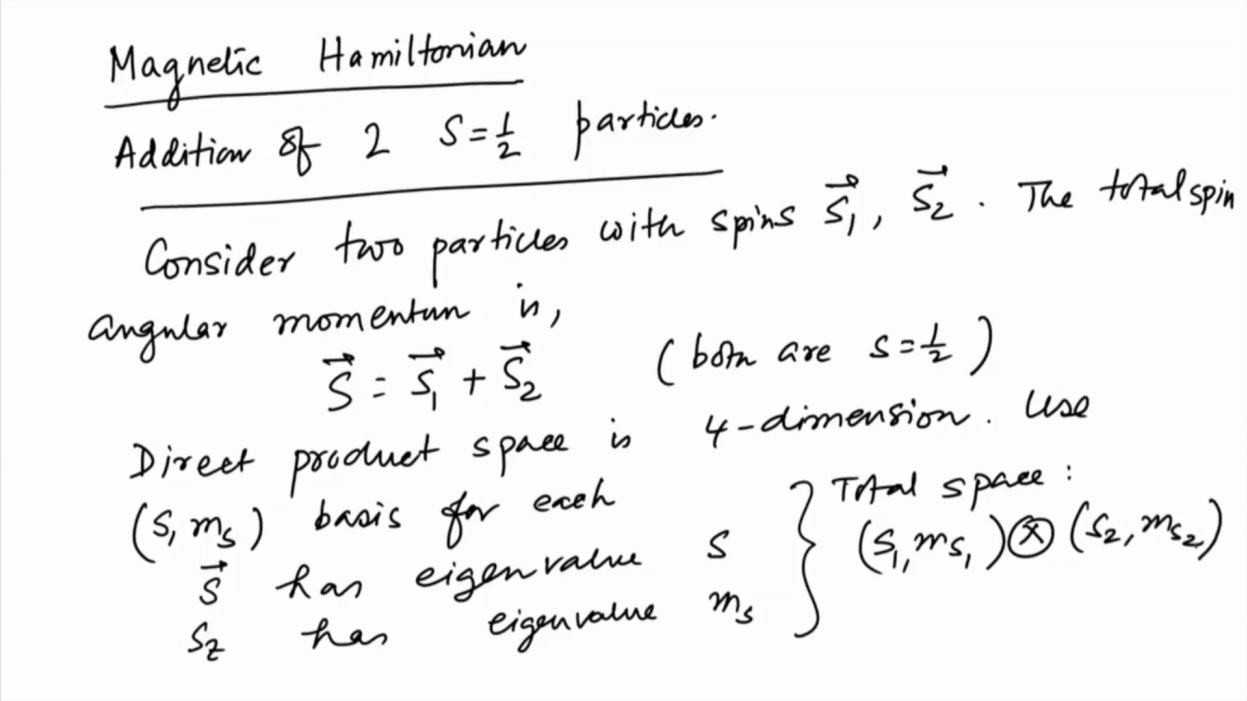


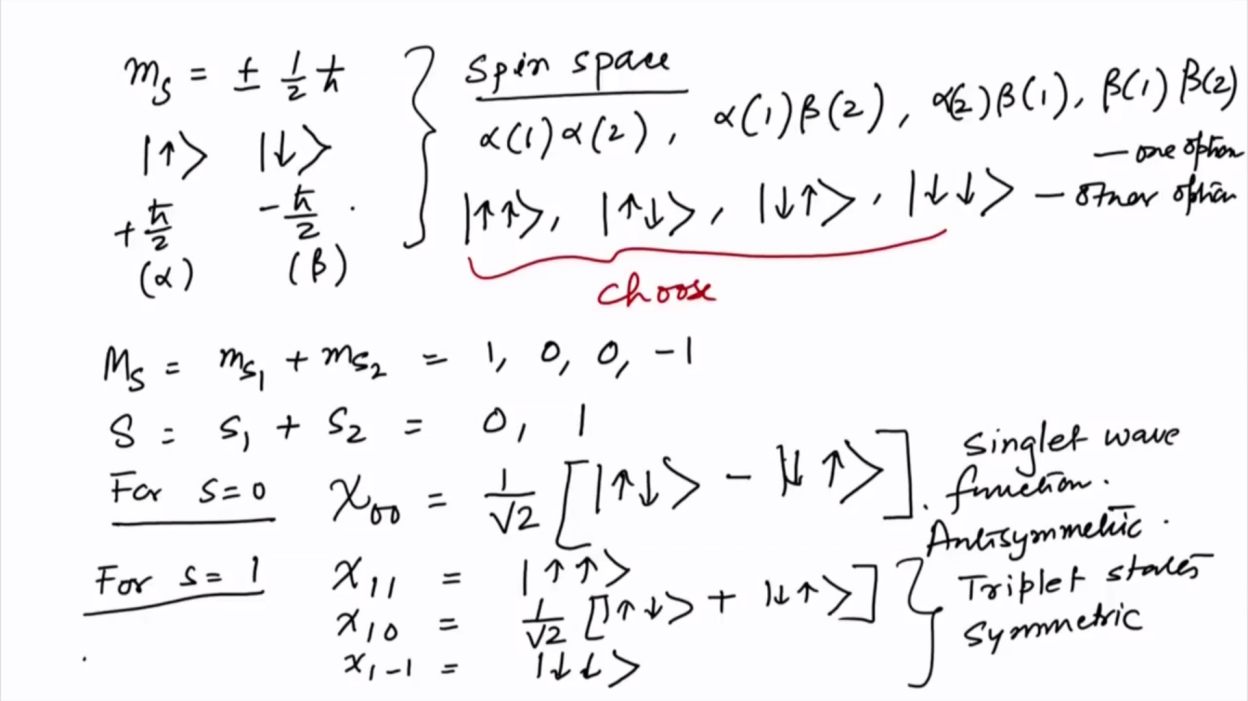
Prof. Saurabh Basu: Let us now discuss how one gets a magnetic Hamiltonian involving only spins. We are particularly talking about Ising kind of Hamiltonians or Heisenberg kind of Hamiltonians. Mainly, we would be talking about Ising Hamiltonians where the spin can only have either pointing up or down.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



So we want to study magnetic Hamiltonian and a derivation of a magnetic Hamiltonian would require that we know the addition of spins. So, say, addition of two spins and these are spin half particles. So we have 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 $S = S_1 + S_2$, where S_1 and S_2 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 that consists of -- it's of four dimensions. So the 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 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 produce of two such S, m_s that is S_1. So total space is (S_1, m_{s1}) x (S_2, m_{s2}).



Let the -- since we have for each one of them, so $m_s = \pm$ ½ ħ, so let's represent the states by ↑ and ↓, so each of these ½ ħ will correspond to say a ↑ and this minus half will correspond to minus half ħ, so +ħ/2 and this is -ħ/2, and hence we'll have -- we can write it in two ways. So the spin space or the direct product space is either you call it α(1), so maybe this is called as α and this is called as a β. So it's α(1) α(2), which means both are in $|\uparrow>$, α(1) β(2) means one of them in $|\uparrow>$ and the other in $|\downarrow>$, and α(2) β(1), the first one is in the down and the second is in up; or both of them are in the down.

This is one option whereas the other option is that we can write it as $|\uparrow\uparrow>$ as a states, $|\uparrow\downarrow>$ and $|\downarrow\uparrow>$, and $|\downarrow\downarrow>$, okay. So this is other option. We can simply choose one of them, but let us choose this option in order to write the wave function and -- I mean to discuss this problem of two spins.

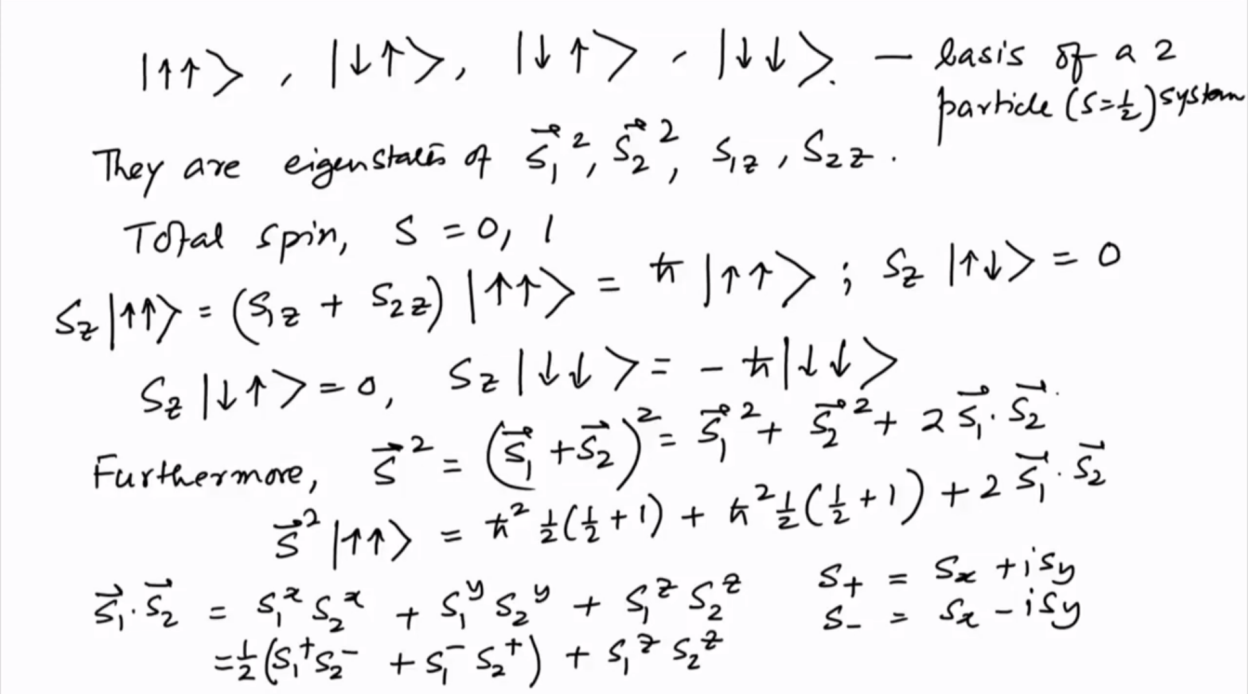
So what is the total value of m_s, which is $m_{s1} + m_{s2}$, which can take value 1, 0, 0, -1; 1 when they both add up ½ + ½ and this is when ½ - ½, this is - ½ ½, and this -½ -½, and the total spin quantum number S, which is equal to $S_1 + S_1$, which can take value 0 and 1, okay. So for S = 0, we have just one eigen function and that eigen function, let's write it with a form which is $|\chi 00>$, which is 1/√2 and I have a $|\uparrow\downarrow - \downarrow\uparrow>$. So 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 downstate. Here, the first one is in downstate and the second one is in upstate, and now if you interchange

↑ to ↓ one gets a negative sign. So that's why it's called as a antisymmetric, and for S=1, we would need -- so for S=1, we'll have three combinations, because we'll have to take care of |χ11>, which will be simply |↑↑> state, |χ10> which will simply be combination of |↑↓+↓↑>, and |χ1-1>, which is equal to a |↓↓> state. Now all these are called as triplets and triplet states, because they are three in number and one can easily check that they are symmetric, because if the first particle is swapped with the second particle, the wave function remains the same.

So these are the state or the wave functions for the two particles, both spin half, and there's a -- for a system consisting or comprising of two spin half particles and all possible combinations have been taken. We get four states and those four states are one singlet and three triplet states. The singlet state is 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 state what about the eigenvalues, because in order to solve a full quantum mechanical problem, we need both the information and the eigenvalues and the eigen functions.



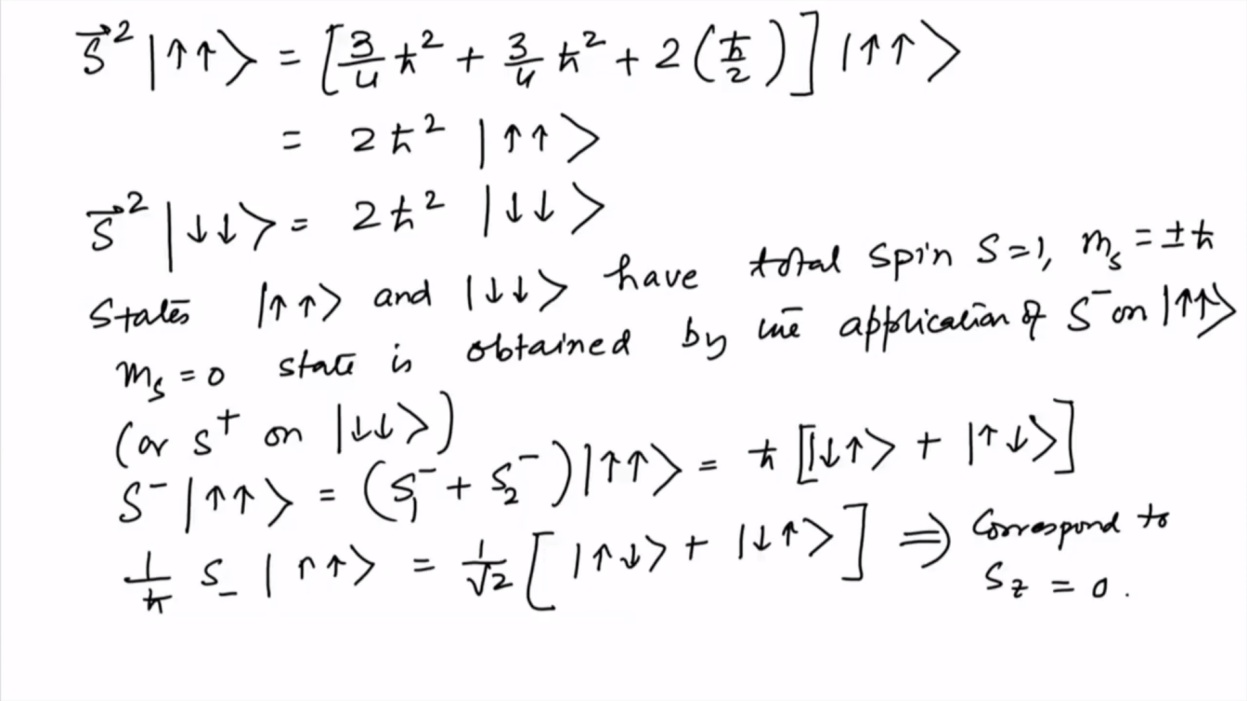
So let us see that, so all these three states, so now we'll talk about the eigenvalues. These states are |↑↑>, |↑↓>, |↓↑>, and |↓↓>, so this forms the basis of the problem of a two-particle spin half system.

So they are eigenstates of S_1^2, S_2^2, S_{1z} and S_{2z}. So the total spin S can be 0 or 1, okay. So now we can see how these total spin operators act on each of these states. So the total spin operator, which $S_z = (S_{1z} + S_{2z})$, that action, the state acting on -- or let us write is here as well. So S_z acting on the $|\uparrow\uparrow>$ state, this will give me S_{1z} will only act on the first spin on the left and S_{2z} will act on the spin on the right. So this will give me $\hbar/2$ for each one of them and $\hbar/2$ and a $|\uparrow\uparrow>$. So as we have said that these are eigenstates of these operators, so I get an eigenvalue equation, which is S_z acting on a $|\uparrow\uparrow>$ state gives me $\hbar/2$ as the eigenvalue and returns me the $|\uparrow\uparrow>$ state as well.

Similarly, for S_z acting on $|\uparrow\downarrow>$ would give me 0, because S_{1z} will give me a $\hbar/2$ and S_{2z} will give me $-\hbar/2$, and similarly we'll also have Sz acting on the state $|\downarrow\uparrow>$ state should also give me 0, and S_z now acting on the $|\downarrow\downarrow>$ state will give me a $-\hbar$ -- sorry there is a $-\hbar/2$ for each so this should be simply $\hbar$. So for each one of them there's an $\hbar/2$, so there are two $\hbar/2$ which makes this $\hbar$. So S_z on $|\downarrow\downarrow>$ will give me a $-\hbar$ and so on. So these are the eigenvalues of this S_z operator.

So furthermore, we have $S_2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1.S_2$, S_1 and S_2 will commute with each other, because they pertain to different particles. So S_1^2 will be $\hbar$ -- so it's ½ (½ + 1), this acting on. So S^2 acting on any of these states, so say we talk about $|\uparrow\uparrow>$, say for example, so this is equal to ½ (½ +1) -- it's S (S + 1), so that is this. Then again, for the S_2^2 this will be ½ (½ +1).

Now we of course don't know what is $2S_1 + S_2$, so we'll leave it for the moment, and let us see that what we can do for the $S_1.S_2$. so $S_1.S_2$ if you see it is equal to $S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z$. Now if you introduce these ladder operators for the spins, so S+ can be written as $S_x + iS_y$ and S- can be written as $S_x = iS_y$. Now this will give me $(S_1+ S_1- + S_1- S_2+)$ and then there'll be a factor of ½ there and $+ S_1^z S_2^z$.



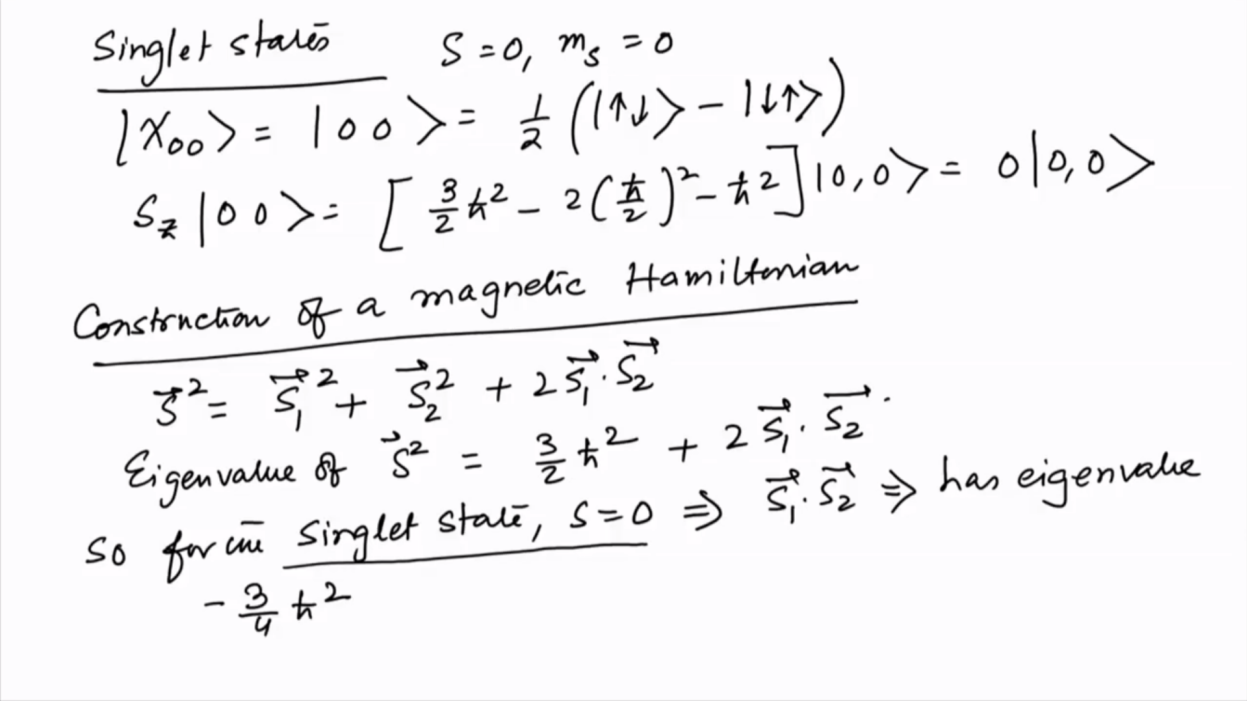
So this is $S_1.S_2$, and hence what we can do is we can see that S_2 acting on a $|\uparrow\uparrow>$, which we have already saw that the first term gives ¾ ħ2, second terms gives ¾ ħ2 as well. Now we have a $2S_1.S_2$. Now for the $|\uparrow\uparrow>$ state, this will raise the sin and hence it will be 0, because up is the maximally aligned state and though S_2- can give you a non-zero contribution, but S_1+ will give 0, and similarly S_2+ will give 0 and that's why these two terms do no contribute, and that simplifies the problems and then we are left with S_{1z} S_{2z}, for which we know the operation. So that's why we have done this, and this is 2(ħ/2) and this whole thing or rather acted upon by this. So it is a eigenvalue equation and this is, if you simplify it, it becomes equal to 2ħ2 $|\uparrow\uparrow>$ and so on

Similarly, for the $|\downarrow\downarrow>$ as well, one gets the same answer by doing the same technique. One gets this as a -- so on these, acting on the $|\downarrow\downarrow>$ state will give us 2ħ2 and a $|\downarrow\downarrow>$. So they have -- so these state $|\uparrow\uparrow>$ and $|\downarrow\downarrow>$ have total spin S=1 and ms = ±ħ, okay.

Of course, S = -1 should have three states, which are equal to $m_s = \pm h$ and 0. So the third state, so $m_s = \pm h$ is there, so $m_s = 0$ state is obtained by a particular operation, so by the application of S- on $|\uparrow\uparrow>$ state. Let's see how one gets it; or you can also consider -- or S+ on the $|\downarrow\downarrow>$ states. So S- on the $|\uparrow\uparrow>$ state gives me S_1- + S_2- on the $|\uparrow\uparrow>$ state, which gives me -- so S_1- 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 eigenstates of $|\uparrow\uparrow>$, but it will operate on this and give me, this S_1 will give me a ħ and will give me a $|\uparrow\downarrow>$ -- sorry it will be a $|\downarrow\uparrow>$. The first one will

lower, so it's a $|\downarrow\uparrow + \uparrow\downarrow>$. S_2 will lower the other one with an eigenvalue which is given by ħ. So 1/ħ S- $|\uparrow\uparrow>$ is nothing but 1/√2, which comes as a normalization factor, $|\uparrow\downarrow + \downarrow\uparrow>$, it doesn't matter we have written down the second term ahead of the first term, and this will correspond to $S_z = 0$. So these three will be called as the triplet states.

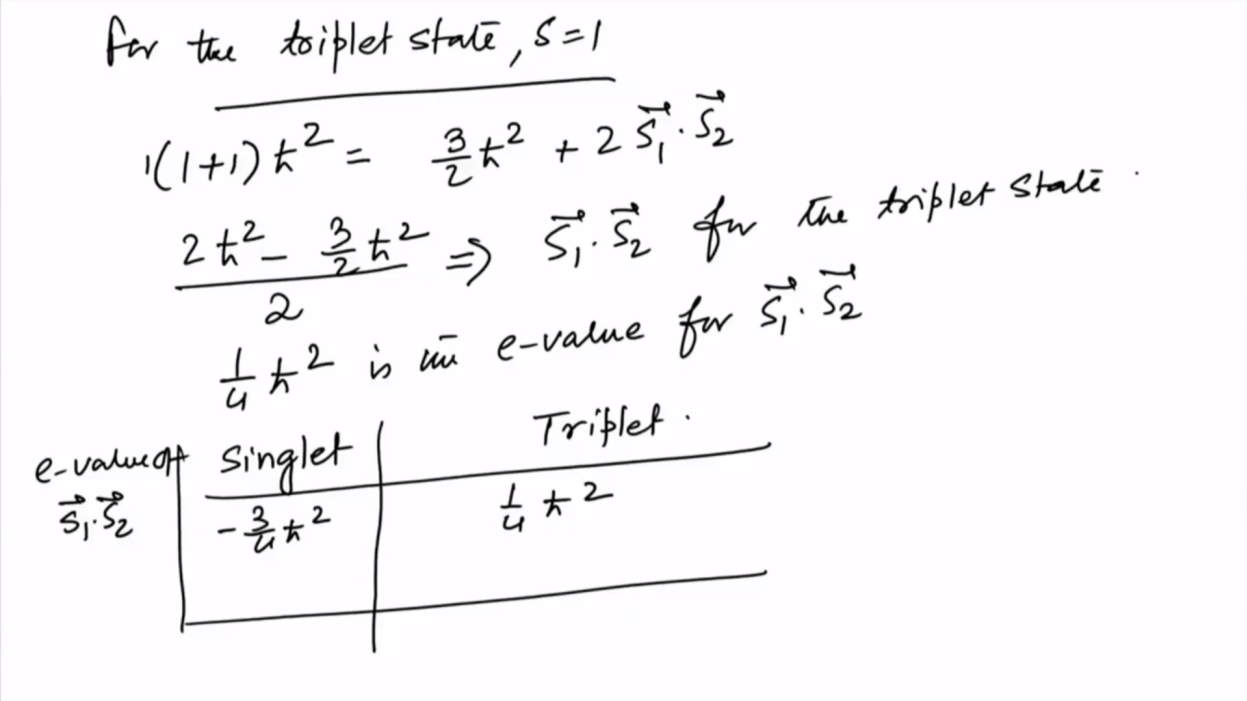
So the singlet states are of course which corresponds to -- so these are the triplet states. So the 2 that's coming over here with spin S = 1 and $m_s = 1$, which is here and the other one comes from here. So these are the three states.



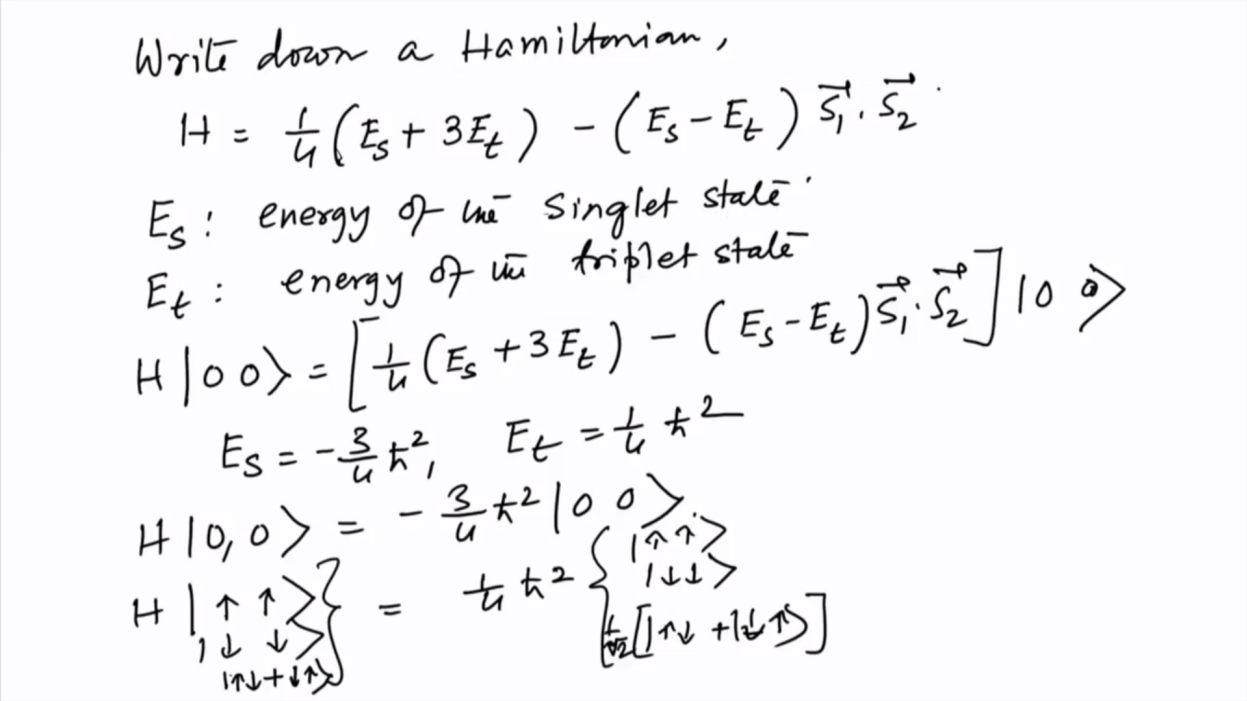
Now we'll just look at the single state, which corresponds to S = 0, $m_s = 0$. Let's just call it as, we can call it as $|\chi 00>$ or we can also use a notation, which is like |00>, which is equal to ½ ($|\uparrow\downarrow - \downarrow\uparrow>$). So why is it a singlet state? So S_z acting on this |00> will give me a 3/2 -- it's $S_{1z} + S_{2z}$ which will act on this, it will be a 3/2 $\hbar^2$ - $2(\hbar/2)^2$ - $\hbar^2$, acting on |00> and it will give me a 0|00>, which means that m_s value of this equal to 0, and this has S = 0. So we have found out all the four eigenstates of this 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, as I said, like a Ising Hamilton or Heisenberg Hamiltonian if h has a full rotational symmetry. So let's just discuss the construction of a magnetic Hamiltonian.

So we have $S_2 = S_1^2 + S_2^2 + 2S_1.S_2$, now the eigenvalue of $S_2 = 3/2\ \hbar^2$, as we have discussed that 3/2 comes from two terms of $¾\ \hbar^2$, each of S_1 and S_2, and plus a $2S_1.S_2$. So for the singlet state, that is S=0, we'll have to put S=0, the $S_1.S_2$ has an eigenvalue, which is equal 2 -½ -3/4 $\hbar^2$, because this is equal to 0. If you put the right hand side equal to 0, the S_1. S_2 will have an eigenvalue which is half of or minus of half of 3/2 ħ2, which is -3/4 $\hbar^2$...

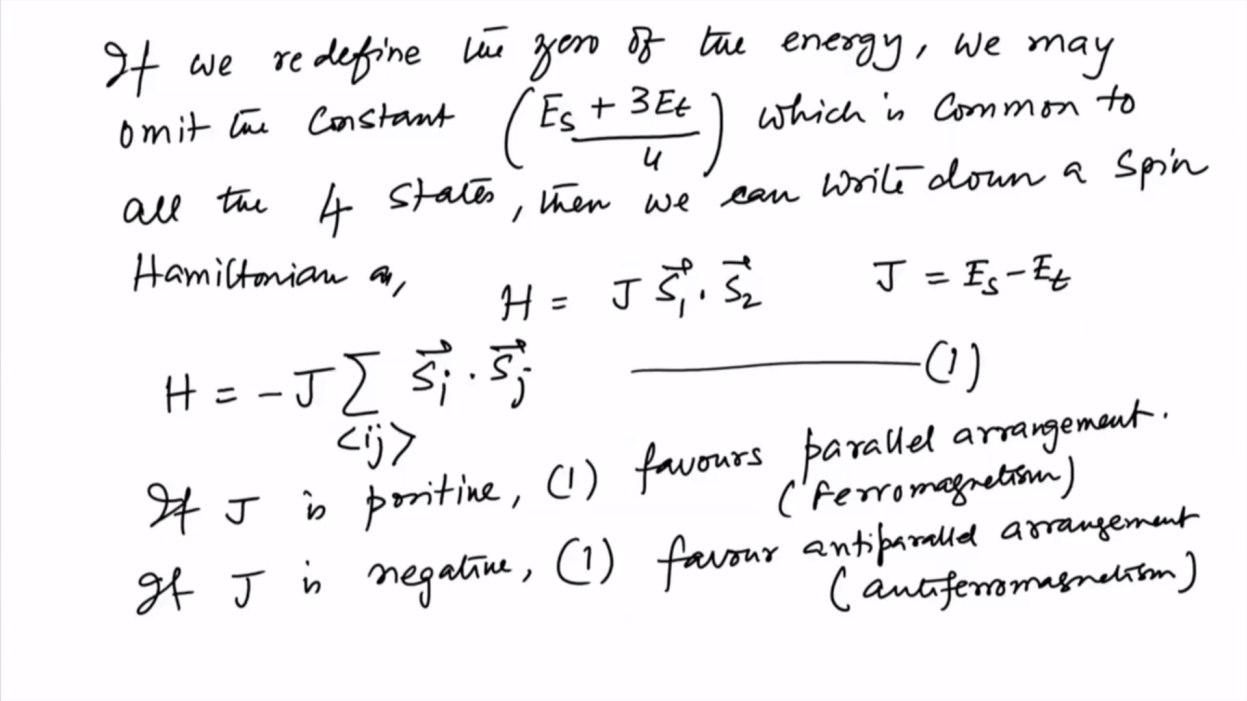


Whereas for the triplet state, which corresponds to S=1, so that will have 1(1 + 1) $\hbar^2$ for the left hand side, which is equal to 3/2 $\hbar^2$ + $2S_1.S_2$, so this is equal to 2, so $2\hbar^2$ - 3/2 $\hbar^2$/2 is the eigenvalue for $S_1.S_2$ for the triplet state. So this is equal to 2 - 3/2 is just ½, so this is equal to ¼ $\hbar^2$. So ¼ $\hbar^2$ is the eigenvalue, in short e-value I am writing, for the operator $S_1.S_2$ for a 2-particle problem. So let's just summarize this quick result. So for singlet states $S_1.S_2$ -- so this is singlet and triplet. So this singlet one has -¾ $\hbar^2$ and this is ¼ $\hbar^2$. So this is the eigenvalue of $S_1.S_2$.



Now if we write down a Hamiltonian, which is $H = ¼ (E_s + 3E_t)$, I'll tell you what these are, $(E_s - E_t)\ S_1.S_2$, we have written it in a particular way of this term where E_s is the energy of the singlet state and E_t is the energy of the triplet state. Why have we written it in this fashion, is that H acting on the single state which is |00> will be simply equal to this $¼ (E_s + 3E_t)$ and $(E_s - E_t)\ S_1.S_2$ acting on |00> -- we can skip the comma in between -- so that's a singlet states. So with $E_s = -¾\ \hbar^2$ and $E_t = ¼\ \hbar^2$, one can simply check that H|00> will give me a $-¾\ \hbar^2$ |00>, and similarly H acting on either of these |↑↑> states or |↓↓> states or |↑↓+↓↑> states, all those multitude of |↓↓> or |↑↓+↓↑> up state with a normalization will give me a $¼\ \hbar^2$ and these states that we have written such as |↑↑>, |↓↓>, |↑↓+↓↑>.

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

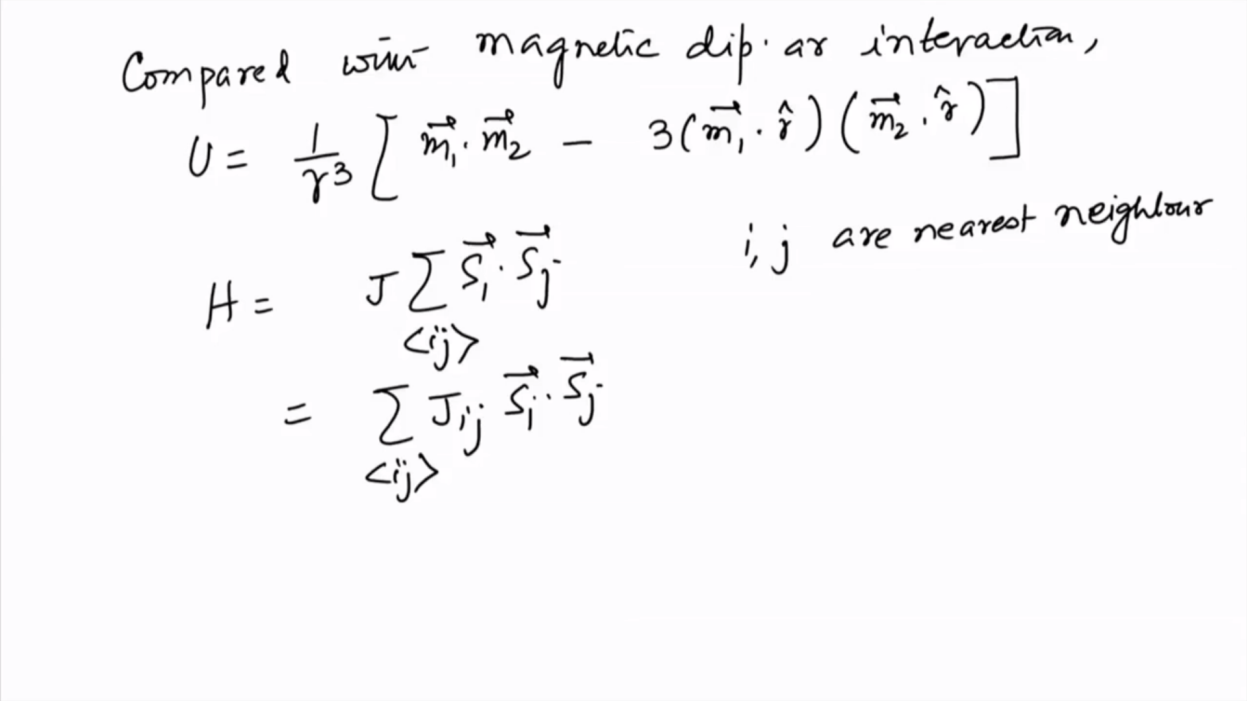


Now we can see that if you redefine the zero of the energy, we may omit the constant (E_s + $3E_t/4$), which is common to all the states, all the four states. Then we can write down a spin Hamiltonian as $H = J\ S_1.S_2$, where J is nothing but the difference between the singlet and the triplet energies. Here of course we have the singlet energy to be lower, which is equal to - ¾ $\hbar^2$ and Et being ¼ ħ2. 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 spin having any values. It should be then -- it's a J and then there is a $S_i.S_j$, it's i and j. It's between the neighboring sites and this is of Heisenberg Hamiltonian, if S has a full rotational symmetry, and it's just the Ising Hamiltonian if S is taken as ±½, but however it gives magnetic properties of the magnetic system such as antiferromagnet or ferromagnet, and of course if J is positive, now we are not restricting ourselves to only two particles where we know that J is negative, but we also go ahead and consider J to be positive as well.

So if J is positive in this particular model, in this Hamiltonian given by (1), (1) favors -- we can write it with a minus sign, putting a minus sign from outside, then this favors parallel arrangements of spins, which are essential for ferromagnetism. And if J is negative, then (1) favors antiparallel arrangement and it is antiferromagnetism. We have seen this phenomena from a purely electronic model, which is Hubbard model, but however, we have also gotten exposed to this kind of spin only models, which are there.

So if J is positive, then the energy is lowered. If the $S_i.S_j$ that is the S_i and S_j, they point, spin point vectors point in the same direction, which are in a sense we talk about ferromagnetism, whereas if J is negative, then that means that whole energy would be negative if S_i and S_j are antiparallelly aligned which are the features of antiferromagnetism.



So this can be actually compared with the magnetic dipolar interaction, like this which is 1/r3 and it's $m_1.m_2$, 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 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 [$S_i.S_j$] has -- there are a large number of approximations that are going on, namely i, j are nearest neighbors. One doesn't have to be, on can include longer than nearest neighbor, that is next to next nearest neighbor interactions as well, and we can also write this inside, the J to be inside and it doesn't have to be constant, and it can be depend from one bond to another. So these are possible Hamiltonians and they have all been explored in the context of spin systems.