Advanced Condensed Matter Physics
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Lecture - 08
Singlet and Triplet States: Magnetic Hamiltonian

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 can derive Hamiltonian which we have introduced or rather we have talked about when we spoke on magnetism during our lectures.

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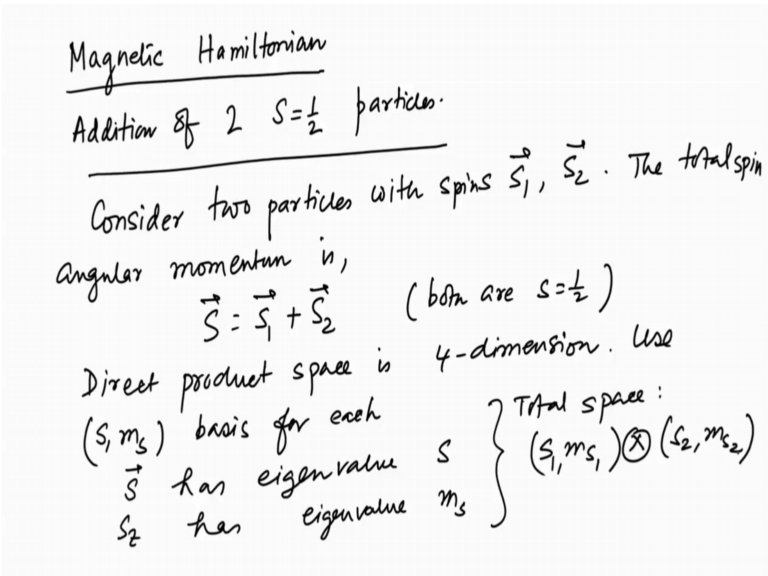

So, to be want to study magnetic Hamiltonian and a derivation of a magnetic Hamiltonian would require that we know the addition of spins or; so say addition of 2 spins, 2 and these are spin half particles. So, we have 2 spin half particles and we would see that how one actually at the spin vectors.

So, let us consider 2 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 2s are the spin vectors for the 2 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 a 4 dimensions. So, the direct product space is 4-dimensional and we can use the bases use S m s basis for each. So, what I mean by that is that the eigen value for the spin operator S is has eigen value S and S z has eigen value 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 2 such S m s that is S 1. So, total product total space is S 1 m s 1 and S 2 m s 2.

(Refer Slide Time: 04:32)

$m_s = \pm \frac{1}{2}\hbar$

$|\uparrow\rangle \quad |\downarrow\rangle$

$+\frac{\hbar}{2} \quad -\frac{\hbar}{2}$

$(\alpha) \quad (\beta)$

Spin space

$\alpha(1)\alpha(2),\ \alpha(1)\beta(2),\ \alpha(2)\beta(1),\ \beta(1)\beta(2)$ – one option

$\underbrace{|\uparrow\uparrow\rangle,\ |\uparrow\downarrow\rangle,\ |\downarrow\uparrow\rangle,}_{\text{choose}}\ |\downarrow\downarrow\rangle$ – other option

$M_s = m_{s_1} + m_{s_2} = 1, 0, 0, -1$

$S = s_1 + s_2 = 0, 1$

For $S=0$ $\quad \chi_{00} = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$. Singlet wave function. Antisymmetric.

For $S=1$

$$\left.\begin{aligned} \chi_{11} &= |\uparrow\uparrow\rangle \\ \chi_{10} &= \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] \\ \chi_{1-1} &= |\downarrow\downarrow\rangle \end{aligned}\right\} \text{Triplet states, Symmetric}$$

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 up will correspond to minus half h cross. So, this h cross over 2 and this is minus h cross over 2

And hence will have we can write it in 2 ways. So, the space the spin space or the direct product space is either you call it alpha 1. So, may be this is called as the alpha and this is called as the beta or so its alpha 1 alpha 2 which means both are in up spin states. Alpha 1 beta 2 means one of them in up spin 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.

Whereas, the other option is that we can write it as up up as the states up down and down up and down down ok. 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 is minus half and this minus half minus half. And the total spins 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 they just one Eigen function and that Eigen function let us write it with the form which is chi is 0 0 which is equal to 1 over root 2 and I have a up down minus a down up.

So, this is this called as the singlet wave function and this is anti symmetric, what I mean by antisymmetric is the following. But, you have 2 particles, so the first one is in upstate and the second one is in down state here the second one the first one is in down state second one was in is in upstate and now, if you interchange up down one gets a negative sign. So, this is that is why it is called as the anti symmetric and for S equal to 1 we would need. So, for S equal to 1 will have 3 combinations because will have to take care of chi 11 which will be simply a up up state chi 10 which will simply be combination of up down plus a down up and a chi 1 minus 1 which is equal to down down state.

Now, all these are called as triplet and triplet states because there are 3 in number and one can easily check that they are symmetric because if the first particle is written swap to the second particle where the function remains the same. So, these are the states or the wave functions for 2 particles both spin half and our for a system consisting of or comprising of 2 spinner particles and all possible combinations have been taken. We get 4 states and those 4 states are 1 singlet and 3 triplet us states the singlet state is the anti symmetric 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 Eigen values, because in order to solve a full quantum mechanical problem we both we need both the information on the Eigen values and the Eigen functions. So, let us see that all these 3 states. So, now, we will talk about the Eigen value 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.

(Refer Slide Time: 10:26)

$|\uparrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$ · $|\downarrow\downarrow\rangle$ — 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, $S = 0, 1$

$S_z|\uparrow\uparrow\rangle = (S_{1z} + S_{2z})|\uparrow\uparrow\rangle = \hbar|\uparrow\uparrow\rangle$; $S_z|\uparrow\downarrow\rangle = 0$

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

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

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

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

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

So, they are Eigen states of S 1 square S 2 square S 1 z and S 2 z. So, the total spin 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 these 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 of them and I will get a h cross by 2 and up up. So, as we have said that these are Eigen states of these operators. So, I get a Eigen value equation which is S z acting on a up up state gives me h cross by 2 as the Eigen value returns me the up up state as 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 will also have S z acting on the down up state should also give 0 and S z now, acting on the down down state will give me a minus h cross sorry this is the minus h cross by 2 for a each of they should be simply h cross. So, this is e for each one of them is an h cross by 2. So, there is a there are 2 h cross by 2 which make a h cross. So, S z on down down will give me a minus h cross and so on.

So, these are the Eigen values of these S z operator and what about; so further more we have 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.

(Refer Slide Time: 16:26)

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

$$= 2\hbar^2|\uparrow\uparrow\rangle$$

$$\vec{S}^2|\downarrow\downarrow\rangle = 2\hbar^2|\downarrow\downarrow\rangle$$

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 the up is the maximally align state and though S 2 minus can give you a nonzero contribution, but S 1 plus will give you 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 a Eigen value equation and this is if you simplify it would becomes equal to 2 h cross square up up and so on. And similarly for the down down as well one gets a same answer by doing the same technique one gets this as. So, on these acting on the down down state will give 2 h cross square and a down down and so they have, these states up up and down down have total spin S equal to 1 and m S plus minus h cross ok. But of course, S equal to 1 should have 3 states which are equal to m S plus minus h and 0.

So, the third states, m S equal to 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 S 2 minus on the up up state which gives me, so S 1 minus will load this spin.

Now, this is something that you should have done in quantum mechanics this gives me an Eigen value which is these are not Eigen states of up up, but I 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 load. So, it is a down up plus an up down S 2 will lower the other one with an Eigen value which is given by h cross. 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 3 will be called as the triplet states and.

(Refer Slide Time: 21:13)

Singlet states $S=0,\ m_s=0$

$$|\chi_{00}\rangle = |0\,0\rangle = \frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$S_z|0\,0\rangle = \left[\frac{3}{2}\hbar^2 - 2\left(\frac{\hbar}{2}\right)^2 - \hbar^2\right]|0,0\rangle = 0|0,0\rangle$$

Construction of a magnetic Hamiltonian

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

Eigenvalue of $\vec{S}^2 = \frac{3}{2}\hbar^2 + 2\vec{S}_1\cdot\vec{S}_2$.

So for the singlet state, $S=0 \Rightarrow \vec{S}_1\cdot\vec{S}_2 \Rightarrow$ has eigenvalue $-\frac{3}{4}\hbar^2$

So, the singlet states are of course which corresponds to, so these are the triplet states. So, the 2 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 3 states and now, will just look at the singlet state which corresponds to S equal to 0 m s equal to 0 let just call it as we can call it as the chi 0 0 or you can use a notation which is like 0 0 which is equal to 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, its 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 4 Eigen states of this of this 2 particle problem.

So, let us now, look at the spin Hamiltonian consisting of the these if you want to construct a Hamiltonian only consisting of the these 2 spins which is like a as I said 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, we have S square which is equal to S 1 square plus S S 2 square plus a 2 S 1 dot S 2. Now, the Eigen value of, Eigen value of S square is equal to 3 by 2 h cross square. As we have discussed that 3 by 2 comes from 2 terms of 3 by 2 h cross square each of S 1 and S 2 and a plus 2 S 1 dot S 2.

So, for the singlet state that is S equal to 0 will have to put S equal to 0 the S 1, S 1 dot S 2 has an Eigen value which is equal to minus half, minus three-fourth h cross square because this is equal to 0 if you put the right hand is equal to 0 the S 1 dot S 2 will have a Eigen value which is half of minus of half of 3 by 2 h cross square which is minus 3 by 4 h cross square.

(Refer Slide Time: 25:35)

for the triplet state, $S=1$

$$1(1+1)\hbar^2 = \frac{3}{2}\hbar^2 + 2\vec{S}_1\cdot\vec{S}_2$$

$$\frac{2\hbar^2 - \frac{3}{2}\hbar^2}{2} \Rightarrow \vec{S}_1\cdot\vec{S}_2 \text{ for the triplet state.}$$

$\frac{1}{4}\hbar^2$ is the e-value for $\vec{S}_1\cdot\vec{S}_2$

	Singlet	Triplet.
e-value of $\vec{S}_1\cdot\vec{S}_2$	$-\frac{3}{4}\hbar^2$	$\frac{1}{4}\hbar^2$

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

So, this is equal to 2 minus 3 half just half. So, this is equal to one-fourth h cross square. So, one-fourth h cross square is the Eigen value in short e value I am writing, for the operator S 1 dot S 2 in the for a for a 2 particle problem. So, they 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 Eigen value of S 1 dot S 2.

(Refer Slide Time: 27:29)

Write down a Hamiltonian,

$$H = \frac{1}{4}(E_s + 3E_t) - (E_s - E_t)\vec{S}_1 \cdot \vec{S}_2$$

E_s : energy of the singlet state

E_t : energy of the triplet state

$$H|0\,0\rangle = \left[\frac{1}{4}(E_s + 3E_t) - (E_s - E_t)\vec{S}_1 \cdot \vec{S}_2\right]|0\,0\rangle$$

$$E_s = -\frac{3}{4}\hbar^2, \quad E_t = \frac{1}{4}\hbar^2$$

$$H|0,0\rangle = -\frac{3}{4}\hbar^2|0\,0\rangle$$

$$H\left\{\begin{array}{l}|\uparrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \\ |\uparrow\downarrow+\downarrow\uparrow\rangle\end{array}\right\} = \frac{1}{4}\hbar^2\left\{\begin{array}{l}|\uparrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \\ \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle\right]\end{array}\right.$$

Now, if we write down 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 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 the 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 Eigen values for a 2 spinner particles for a system of 2 spinner particles and this is that Hamiltonian.

(Refer Slide Time: 30:57)

If we redefine the zero of the energy, we may omit the constant $\left(\frac{E_s + 3E_t}{4}\right)$ which is common to all the 4 states, then we can write down a spin Hamiltonian as,

$$H = J\,\vec{S}_1 \cdot \vec{S}_2 \qquad J = E_s - E_t$$

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad \text{———— (1)}$$

If J is positive, (1) favours parallel arrangement. (ferromagnetism)

If J is negative, (1) favour antiparallel arrangement (antiferromagnetism)

Now, you can see that if you, if you redefine the 0 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 a 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 lowered which is equal to minus 3 by 4 h cross square and E t being one-fourth h cross square. So, J will be negative. Now, if we if we say that such Hamiltaonian's can be written for n particles with the pair wise interaction between the particles then we can write the generic Hamiltonian for a magnetic system or spin half system we can extend it to spin having any values it should be then it is a J and then there is a S i dot S j, its i and j it is between the neighboring sites.

And this is Heisenberg Hamiltonian if S has the full rotational symmetry and it is just the ising Hamiltonian if S is taken as plus minus half ah, but however, it gives magnetic properties of the magnetic systems such as anti ferromagnet or ferromagnet. And of course if J is positive now we are not restricting ourselves to only 2 particles, where we know that J is negative ah, but we also consider go 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 the minus sign putting a minus sign from outside then this favors parallel arrangements of spins and which are essential for ferromagnetism. And if J is negative then 1 favors anti parallel arrangement and it is anti ferromagnetism is.

We have seen these phenomenon from the purely electronic model which is Hubbard model, but; however, we have also got an exposed to this kind of spin only models which are, 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 n j is they point the spin vectors pointing the same direction which are in the sense we talk about ferromagnetism where as if j is negative then; that means, that the whole energy would be negative if S i and S j are anti parallelly, aligned which are the features of anti ferromagnetism 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 2 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 ah, but here we have a purely spin Hamiltonian which neglects all spatial symmetries.

(Refer Slide Time: 35:48)

Compared with magnetic dipolar interaction,

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

$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j \qquad i, j \text{ are nearest neighbour}$$

$$= \sum_{\langle ij\rangle} J_{ij}\,\vec{S}_i\cdot\vec{S}_j$$

Now, this is H written as J, S i dot S j has there are a large number of approximations that are going on namely i j's are the nearest neighbors one does not have to be one can include longer than nearest neighbor that is next to next nearest interactions as 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 one bond to another and so these are, these are possible Hamiltonians and they have all been explored in the context of spin systems.