NMR Spectroscopy for Chemists and Biologists
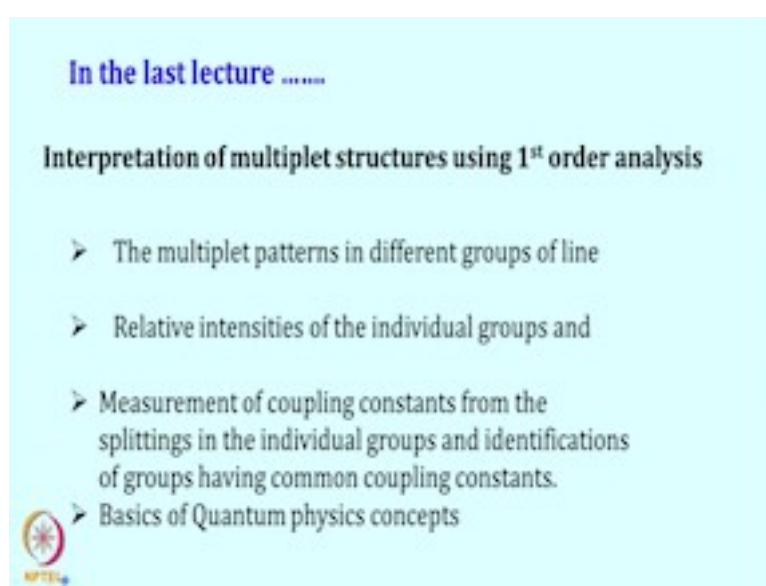**Doctor Ashutosh Kumar**
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Lecture No. 11
Quantum Mechanical Analysis – Part II

Okay, so welcome to today's class we are still discussing about high resolution NMR spectra of molecules.

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In the last lecture ....

Interpretation of multiplet structures using 1st order analysis

➤ The multiplet patterns in different groups of line

➤ Relative intensities of the individual groups and

➤ Measurement of coupling constants from the splittings in the individual groups and identifications of groups having common coupling constants.

➤ Basics of Quantum physics concepts

In the last lecture we started with the explanation of interpretation of multiplet structures using first order analysis and then we look in it these multiple patterns in different groups of line how it arises, what could be the basis of relative intensity that is what we started with and measurement of coupling constant from these splitting of individual group and that helps in identification of different groups having the coupling constants and then we started looking at to the basics of quantum physics concepts, we looked at various terms like what is the operator, what is Eigen function, Hamiltonian and Eigen values.

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So actually we were at the state where we wanted to discuss the two spin system like a, let us consider a *AB* system, *AB* case like two spins which have a close proximity of chemical shift and that is what we define as a *AB* system. So both of these spins let us consider they are half spin so I is half for both of these spins, then for such spins we can write the so angular momentum $I = \frac{1}{2}$ and then we can write the Hamiltonian which will be given by these terms

$$H=\frac{1}{2\pi}\left[\gamma_1 H_1 I_{z1}+\gamma_2 H_2 I_{z2}\right]+J I_1 . J I_2$$

Where, γ is the gyromagnetic ratio of spin 1, the H_1 is the Hamiltonian corresponding to that and I_{z1} is the Eigen function for spin number 1.

Now similarly these terms are for spin 2 and then there is a term which arises because of these two spins are coupled and therefore *J* is the coupling constant between these two spins. So total Hamiltonian if these two spins are coupled through bond will be given by these term overall where the contribution from first term is this, second term is this and then because of the coupling between these two terms is a actually JI_1I_2.

So if you look at the resonance frequency of these two will be given by frequency of 1 frequency of 2 and this is coming because of the these two spins are coupled through the bond. So this is Hamiltonian, resultant Hamiltonian for a system two spin system both having half spin. So now for such system we can write the basis set for

for four product function as these like as we said that two spins are there so both either can be in $\alpha\alpha$ state that is one basis set the another basis set can be both one is in α state another is in β state, the third one is β state α state and fourth one is in $\beta\beta$ state.

To simplify that I, let me draw this so we define as say $\alpha\alpha$ state so this is $\alpha\alpha$ both states having of spin, one is α and the another is β like $\alpha\beta$ spin or it can be $\beta\alpha$ spin and then other can be here $\beta\beta$ spin. So these are four basis set and these functions are orthogonal that means if you take product of this $\alpha\alpha\alpha\beta$ one can write it like this

$$¿\alpha\alpha|\alpha\beta \geq ¿\alpha|\alpha> ¿\alpha \vee \beta> ¿0$$

ok so these are the two spin system case.

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Then we can go and define the Eigen function for this operator I_z α β Eigen function for operator I_z and one can calculate the element matrix and if you calculate we get these these term H_{11} and then we can solve this equation so we get essentially the frequencies term here and the coupling term here.

$$H_{11}=¿\alpha\alpha|H|\alpha\alpha \geq v_1 <\alpha|I_{z1}|\alpha> ¿\alpha|\alpha> + v_2 <\alpha|I_{z2}|\alpha> ¿\alpha|\alpha> + J <\alpha\alpha|I_{x1}I_{x2}+I_{y1}I_{y2}+I_{z1}I_{z2}|\alpha\alpha> ¿$$

$$¿\frac{(v_1+v_2)}{2} + J\{<\alpha\alpha|I_{x1}I_{x2}|\alpha\alpha> + ¿\alpha\alpha|I_{y1}I_{y2}|\alpha\alpha> + ¿\alpha\alpha|I_{z1}I_{z2}|\alpha\alpha>\}$$

This equation by something called matrix element I_x and I_y by by making use of the raising and lowering operator this is typically used in the quantum mechanics to solve such equation

$$I_x = I^{+¿+\frac{I^{-¿}}{2}}, I_y = I^{+¿+\frac{I^{-}}{2}¿}¿¿ \quad ¿$$

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So if we go ahead and solve this equation what we can find it for these operators following property will arise that means $I^{+}\lvert\alpha\rangle = 0$, and $I^{+}\lvert\beta\rangle = \lvert\alpha\rangle$, so this is like this lowering and raising operator so this is raising operator so that means β will be raised to α state and here it is a lowering operator so α will be lowered to β state. So like say up state that is α state will be lowered by this lowering operator to β state and here I^{+} is applied to β state.

So this is say β state and it will be raised to by raising operator to α state, so that is what, so one can calculate now

$$H_{11} = \frac{\left(v_{1} + v_{2}\right)}{2} + J\left(0 + 0 + \frac{1}{4}\right) = \frac{\left(v_{1} + v_{2}\right)}{2} + \frac{J}{4}$$

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Other elements of matrix

$\mathcal{H}_{12} = 0; \ \mathcal{H}_{13} = 0; \ \mathcal{H}_{14} = 0$

$\mathcal{H}_{21} = 0; \ \mathcal{H}_{22} = \dfrac{(v_1 - v_2)}{2} - \dfrac{J}{4}; \ \mathcal{H}_{23} = \dfrac{J}{2}; \ \mathcal{H}_{24} = 0$

$\mathcal{H}_{31} = 0; \ \mathcal{H}_{32} = \dfrac{J}{2}; \ \mathcal{H}_{33} = \dfrac{(v_2 - v_1)}{2} - \dfrac{J}{4}; \ \mathcal{H}_{34} = 0$

$\mathcal{H}_{41} = 0; \ \mathcal{H}_{42} = 0; \ \mathcal{H}_{43} = 0; \ \mathcal{H}_{44} = -\dfrac{(v_1 + v_2)}{2} + \dfrac{J}{4}$

Similarly, one can calculate the other terms of the matrix so here the other term H_{12} will be 0, H_{13} again will be will be 0, H_{14} will be 0 and if you look at here the point two pay attention the $H_{22} = \dfrac{(v_1 - v_2)}{2} - \dfrac{J}{4}; \ H_{23} = \dfrac{J}{2}$

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The matrix representation of the Hamiltonian in the product basis

$$\mathcal{H} = \begin{bmatrix} \frac{(v_1 + v_2)}{2} + \frac{J}{4} & 0 & 0 & 0 \\ 0 & \frac{(v_1 - v_2)}{2} - \frac{J}{4} & \frac{J}{2} & 0 \\ 0 & \frac{J}{2} & \frac{(v_2 - v_1)}{2} - \frac{J}{4} & 0 \\ 0 & 0 & 0 & -\frac{(v_1 + v_2)}{2} + \frac{J}{4} \end{bmatrix} \quad \begin{matrix} \text{Spin states} \\ \alpha\alpha, \\ \alpha\beta \\ \beta\alpha \\ \beta\beta \end{matrix}$$

One can block diagonalised this matrix to get the eigenvalues of the Hamiltonian

So if you solve this equation we get this block diagonalised representation of this matrix where these are the four elements that we are getting it,

$$
\begin{pmatrix}
H_{11} & H_{12} & H_{13} & H_{14} \\
H_{21} & H_{22} & H_{23} & H_{24} \\
H_{31} & H_{32} & H_{33} & H_{34} \\
H_{41} & H_{42} & H_{43} & H_{44}
\end{pmatrix}
$$

So these are the spin states that we are talking, here is for $\alpha\alpha$, this one for $\alpha\beta$, this is for $\beta\alpha$ and $\beta\beta$ state, so these four states we can represent our Hamiltonian in simplifies form in block diagonalize form to get the Eigen value of these Hamiltonian.

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So okay if we do that and then we can write the Eigen value coming from solving of these equation so we get four Eigen values one for state one that is $\alpha\alpha$ state here and then we have for $\alpha\beta$ state, $\beta\alpha$ state and $\beta\beta$ state so these four state that we are talking in our previous slides, these four states we are getting the Eigen value of these states.

Now Eigen functions of these states one can write

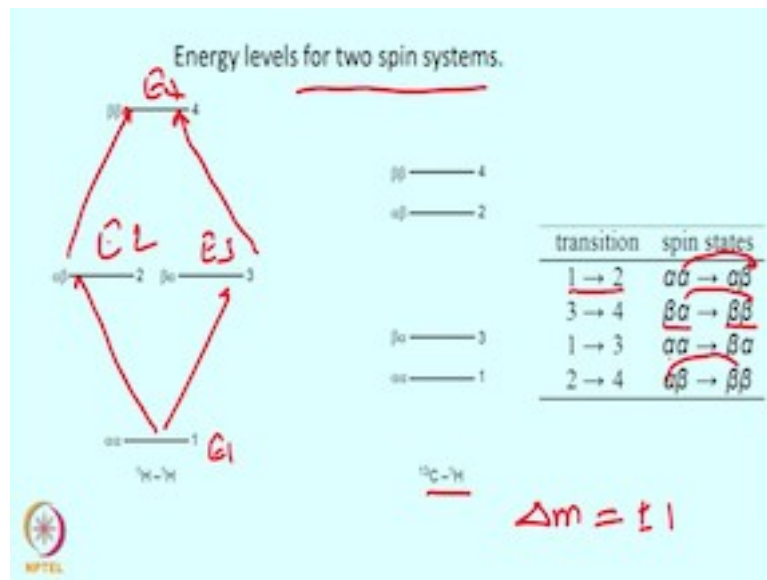$$ H|\alpha\alpha> ¿ E1|\alpha\alpha> H|\beta\beta> ¿ E4|\beta\beta>; \psi1=¿\alpha\alpha>, \psi4=¿\beta\beta>¿ $$

we get the Eigen value is *E1* and similarly for the other state *E2, E3* and *E4*, so

$$ \psi2=\cos\vartheta\alpha\beta>+¿\sin\vartheta\beta\alpha\,¿ $$

$\psi 3 = \sin \vartheta \alpha \beta > + \cos \vartheta \beta \alpha$

So one can solve these and these two terms are coming because these two spins are mixing because of the coupling between them, so 2, 3 terms are coming because of the mixing of the states.

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So these are the sates so as we define, so let us take a simplified version of this. So here we are talking the energy level coming because the states and in the previous slide we calculated $E1, E2, E3$, and $E4$ so where are those, here so $\alpha\alpha$ state say give gives $E1$ and here we have $E2$ and say E3 and $E4$, so these are states $\alpha\alpha$ for H-H coupling, here one can take it also carbon proton but this is not AB system but anyhow here this is the kind of 4 states that we are giving.

So here in this case now we define the 4 energy states for the system. Now as we know that these transitions that will happen between these system will follow these selection rule and selection rule in this case that $\Delta m = \pm 1$, so that means transition will happen $1 \rightarrow 2$ here 1 state 2 state to and that means that this transition will be $\alpha\alpha$ to $\alpha\beta$ state means here second spin is flipping.

The next transition we are talking is $3 \rightarrow 4$. So in this case what is happening $\beta\alpha$ changing to $\beta\beta$. So here again second spin is flipping so this flip is happening, here again this flip is happening so these are the two states and now for these the other spins $1 \rightarrow 3$ transition and the $2 \rightarrow 4$ transition is happening, so in this case $1 \rightarrow 3$

transition $\alpha\alpha$ first spin flips to β and here again $\alpha\beta$ here first spin, here first spin flips to beta states, so the spins that flips is called active spin and spin that does not flip is called passive spin.

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Now let us go back, so the extent of these spin as we saw that it has a J term in the previous slide we looked at it has the energy level has a J term. So the extent depends upon the relative magnitude of the coupling constant. How much coupling constant is there and what is the separation between the chemical shift of these spins so $\frac{J}{\delta}$, J is the coupling constant and δ is the difference in the chemical shift.

So larger the $\frac{J}{\delta}$, $\frac{J}{\delta}$ again I am telling you it is a ratio of coupling constant with the separation in the chemical shift, so stronger then mixing will be stronger so the mixing of 2 spins will be stronger and if it is less then it will be lesser. So if $\frac{J}{\delta}$ 1 this is called a strong coupling case and if $\frac{J}{\delta} \ll 1$ it will be called week coupling system. So AB kind of a strong coupling system because here the shift, the difference in the chemical shift is small however AX kind of a system is called weak coupling system, here the separation in these two chemical shift is quite a bit.

Let us calculate intensity of different transitions :

Ψ2→ Ψ1,Ψ4→ Ψ2,Ψ3→ Ψ1,Ψ4→ Ψ3

Now we know the energy of these states, now we know the Eigen function of these sates and where transitions are happening and what is the probability of transition that one can calculate, so then one can calculate the one can get the frequency value of each of these transition that we talked about and what will be the relative intensity of these transition in various case. So say transition 3 → 1 that we defined in the previous slide 3 → 1 is like here, one of these 1 → 3 or 3 → 1 here, so that transitions will give us the frequency like this where C is a constant.

$$3 \rightarrow 1 = \frac{(v_1 + v_2)}{2} + \frac{J}{2} + C = 1 - \sin 2\theta$$

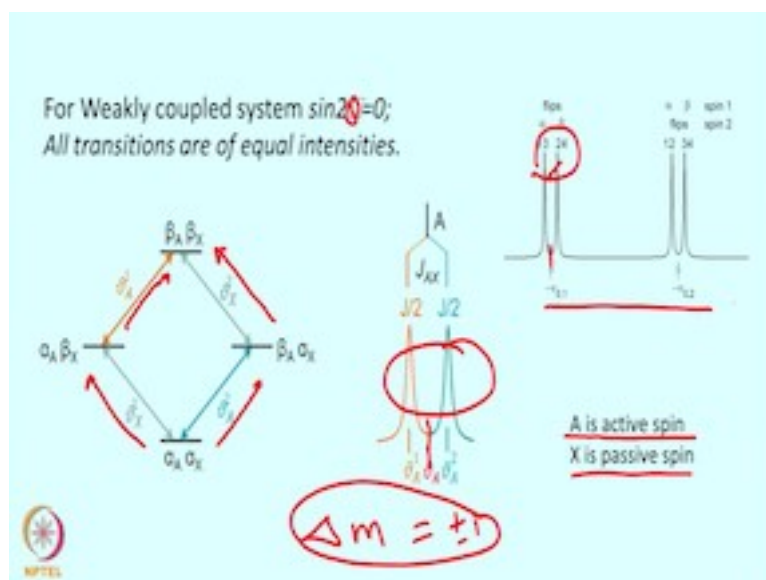$$4 \rightarrow 2 = \frac{(v_1 + v_2)}{2} - \frac{J}{2} + C = 1 + \sin 2\theta$$

$$2 \rightarrow 3 = \frac{(v_1 + v_2)}{2} - \frac{J}{2} - C = 1 - \sin 2\theta$$

$$4 \rightarrow 2 = \frac{(v_1 + v_2)}{2} - \frac{J}{2} + C = 1 + \sin 2\theta$$

$$\sin 2\theta = \frac{J}{2C} = \frac{1}{\sqrt{\delta^2 + J^2}} = \frac{1}{\sqrt{1 + \left(\frac{\delta}{J}\right)^2}}$$

So for these transitions as we mentioned sin 1 to sin2 to sin 3 to sin 4 transition one can get the frequency that comes and get the relative intensity that coming because of these transitions.

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So as we looked at for weak couplings system $\sin 2\theta = 0$,that means all the transitions are going to be of equal intensity. We go back here and if $\sin 2\theta = 0$,that means we are going to get 1, 1, 1, 1 value. So that means for weak coupling system something transitions happening like this therefore transitions that we were discussing a minute ago, now $1 \rightarrow 3$ transition, $2 \rightarrow 4$ transition, $1 \rightarrow 2$ transition or $3 \rightarrow 4$ transition in each of the case intensity is going to be equal and the actually the chemical shift centre will be of say spin 1.

So in this case α flips, here β flips, in this case α flips and β flips. So these spins 1 and 2 this will be case for equal intensity and that is the case for weak coupling system as we have shown earlier. So here we are talking about spin 1 for both of these case and the equal intensity pattern will come. So here will be the centre for frequency 1.

Now A will be called active spin because this spin is flipping in this spectrum and X will be called passive spin this spin is not flipping. If you look at here whatever transition we are seeing here either this transition or this transition or even this transition or this transition what is happening here, our $\Delta m = \pm 1$,either this transition or this transition this is allowed transition in NMR according to selection rule.

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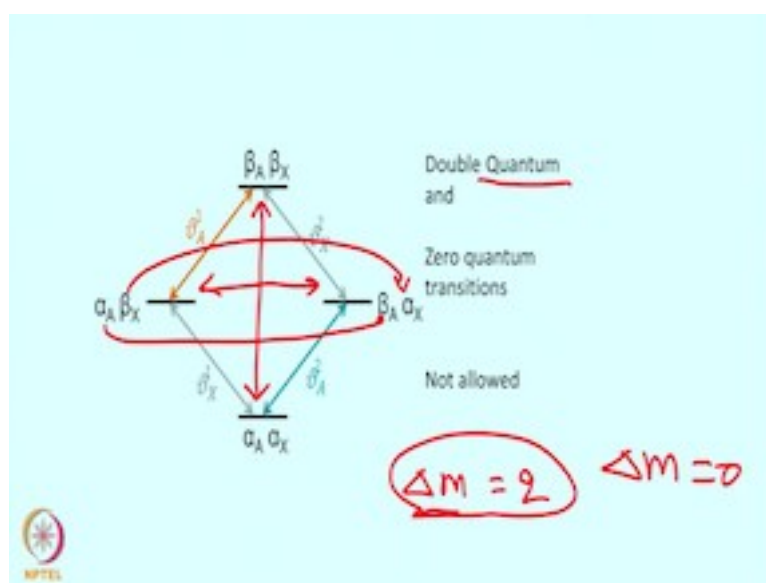
Now this is not only transition that is possible. Some there are some other transition that is possible so one of these transitions can be something like this, say this transition. Now what this transition is, what is happening here, actually both spin A and X are going from $\alpha\alpha$ state to $\beta\beta$ both spin are flipping that means the $\Delta m = 2$. This transition is called double quantum transition.

Two quantum, one from spin number 1, another from spin number 2 both are flipping so that is called double quantum transitions and there another type of transition can also possible like here. Here first A spin is flipping and also the X spin is flipping, since now this is happening both spins are flipping so this is called zero quantum transition because there is no resultant delta so $\Delta m = 0$.

Now this is zero quantum transition so generally double quantum transition or zero quantum transitions are not allowed. So you remember this is not an allowed transition, double quantum transition or zero quantum transition in NMR however using some trick one can exploit this transition. So these are generally called forbidden fruit of NMR spectroscopy and there is some benefit of that because of relaxation parameter that again we will come later.

Now coming back to the intensity parameter so as we discuss few slides back here that θ parameter so we looked at $\sin 2\theta = 0$, that means this is a weak coupling system and all intensity of all four transitions are of equal intensity but suppose it is not 0 then what will happen.

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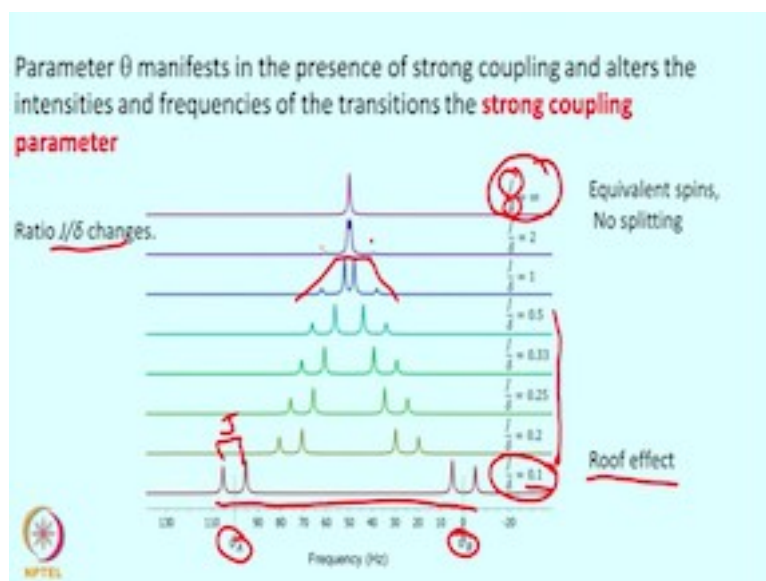
So the parameter theta manifest the presence of strong coupling and then that alters the intensity of frequency of the transitions. So now we have like simulated this spectrum so if you say the ratio of J/δ changes then the intensity and the pattern changes.

Now let us start with a simply like $\frac{J}{\delta}=\infty$, that means $J \gg \delta$ so that that is why we are having infinity value. Now for such case we get a single transition what I mean is J is very large compared to difference in the chemical shift that means they look like or they are the equivalent spins and therefore no splitting will happen. So they are called magnetically equivalent spin where there is no splitting happen.

Now as we start changing here the ratio $\frac{J}{\delta}=2$. You see the splitting pattern starts originating. Now this will split into 2 very small here and then there are two other that are coming here. Now if the chemical shift difference and J becomes equal then we get a 4 peaks 2 central transition peaks are very like very intense compared to the two outer one as we start decreasing this ratio as we go from 0.5 to 0.33 to 0.25 to 0.1.

We see this separation is now changing and here are the two centre so this is the case of weak coupled spin ok. So here the chemical shift difference is ten times more than the coupling constant then peaks will be like this, two spins separated and now this is

the J value between these two and these are the resonance frequency of A spin and B spin.

So this is weak coupling spin, this is magnetically equivalent spins, rest other are for strongly coupled spin as we go from here to here the effect are pronounced and the outer peaks becomes more intense and the central peaks get less intense. So is you look at the pattern of these splitting they have a something like a roof effect. So this is coming because of the strong coupling case this is called roof effect of the splitting and this arises because of strong coupling in the AB system.

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So that what we discussed as $\frac{J}{\delta} = \infty$ that means two spins are equivalent and the outer two transition would have identical 0 intensity and inner two transition would have same energy so the coupling between equivalent spin does not lead to splitting in the NMR spectrum so like if you look at CH_3 in methanol so it will have like for these actually these are equivalent spin and they will have only one peak. So they are magnetically equivalent spins and does not cause splitting of the line in NMR spectrum.

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Summary

Effect of strong coupling :
i)   the spins lose their identity; the transitions cannot be described to a particular spin
ii) the transitions will have different intensities

i)   the product functions corresponding to the same total z-component of spin get mixed ✓

i)   the chemical shifts of the spins cannot be determined by simple inspection of the spectra

To summarize what we saw that what is the effect of strong coupling because of the strong coupling spins looses their identity and the transitions cannot be described to a particular spin system so the analysis in this case becomes little complicated. The transition will have a different intensity as we saw in the previous slides.

Because of a strong coupling, there are two outer peaks are of small intensity and two inner peaks are of greater intensity and the product function corresponding to the same total value of J component that get mixed. So that is case also called strong coupling and the chemical shift of spin cannot be determined by simple inspection of the spectrum, it requires more rigorous analysis. That is what the effect of strong coupling like AB spin system.

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So now we look at the two spin system. Now we move to next NMR spectrum for three coupled spin system, so let us take three coupled spin system where say spin 1, 2 and 3, they can be coupled in two manners, one manner can be *A* is couple to *B* and coupled to *C* or one can if they are weakly coupled we can say *A* is coupled to *M* couple to *X*, the another case will be cyclic, 3 coupling constant here, A will be coupled to *B* and *B* is coupled to *C* and *C* is coupled to *A* so all are coupled to each other.

Now these two can be possibility for three spin system so all spins may be non-equivalent and weakly coupled like as we say weak couple system we can define as a *AMX* system or it can be two spins may be equivalent and weakly coupled or strongly coupled to third spin so say these are say AB_2 kind of system. Now third case can be all spins may be non equivalent, two of them may be strongly coupled so *AB*, *ABX* and here we can have AB_2 kind of system and the last one all three spins may be non equivalent and strongly coupled so that will be *ABC* kind of system.

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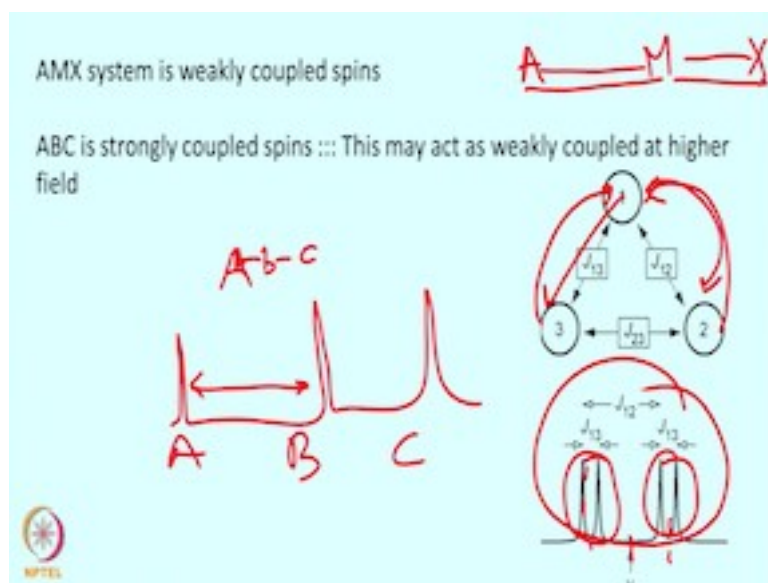
So *AMX* system as we defined is weakly coupled spin so again to remind you what we mean by *AMX* system like their chemical shift if you look at *A* comes here *M* comes here and *X* comes here that is why their chemical shift is separated and that is why we called *AMX* system. On the, on contrary *AB* system is strongly coupled system so this may act to weakly coupled system at higher field so *AB* system that what we mean that in the chemical shift range *A* is coupled to *B* is coupled to *C* but this is say at one field what will happen at the higher field.

If you put the higher field *A* will be here, *B* will be here and *C* will be here, so now they will start behaving like a weakly coupled system. So if they are weakly coupled system then what will happen that each one split so here first say so there are three spin as we described 1, 2, 3. So first this spin is splited because of 1-2 coupling so here are that coupling and then they are splited because of 1-3 coupling so resultant are four lines for say spin number 1, spin number 1 now splited into 4 first because of 1-2 coupling and then because of 2-3 coupling but this is the case for the weakly coupled system.

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Eigenvalues and Eigenfunctions in an AB2 system

S.No	Eigen function	Energy
1	$\alpha\alpha\alpha$	$\frac{1}{2}\nu_A + \nu_B + \frac{1}{2}J_{AB} + \frac{1}{4}J_{BB}$
2	$\alpha(\alpha\beta + \beta\alpha)/\sqrt{2}$	$\frac{1}{2}\nu_A + \frac{1}{4}J_{BB} + M_+$
3	$\beta\alpha\alpha$	$-\frac{1}{2}\nu_A + \nu_B - \frac{1}{2}J_{AB} + \frac{1}{4}J_{BB} - M_+$
4	$\alpha\beta\beta$	$\frac{1}{2}\nu_A - \nu_B - \frac{1}{2}J_{AB} + \frac{1}{4}J_{BB} + M_-$
5	$\beta(\alpha\beta + \beta\alpha)/\sqrt{2}$	$-\frac{1}{2}\nu_A + \frac{1}{4}J_{BB} - M_-$
6	$\beta\beta\beta$	$-\frac{1}{2}\nu_A - \nu_B + \frac{1}{2}J_{AB} + \frac{1}{4}J_{BB}$
7	$\alpha(\alpha\beta - \beta\alpha)/\sqrt{2}$	$\frac{1}{2}\nu_A - \frac{3}{4}J_{BB}$
8	$\beta(\alpha\beta - \beta\alpha)/\sqrt{2}$	$-\frac{1}{2}\nu_A - \frac{3}{4}J_{BB}$

$$M_\pm = \frac{1}{2}([\delta_{AB}^o \pm \frac{1}{2}J_{AB}]^2 + 2J_{AB}^o)^{1/2} - \frac{1}{2}[\delta_{AB}^o \pm \frac{1}{2}J_{AB}]$$

Now let us get this system here like a two spins will be equivalent and weakly or strongly coupled to the third spin so this kind of a AB_2 system. If you write Eigen function and energy for such case using same quantum mechanical trick that we discussed few minutes back. So now what we get is here AB system so two these spins are equivalent and they are strongly coupled to a system so what we have is half of frequency of A then B and then because of mixing of AB and 1 by 4 of BB that is one Eigen function then we have another Eigen function so here frequency of A and coupling constant between BB and so and so far one can write it so here

$$M \pm = \frac{1}{2} ¿$$

NMR spectra for a AB2 spin-system $J_{AB}=10$ Hz).
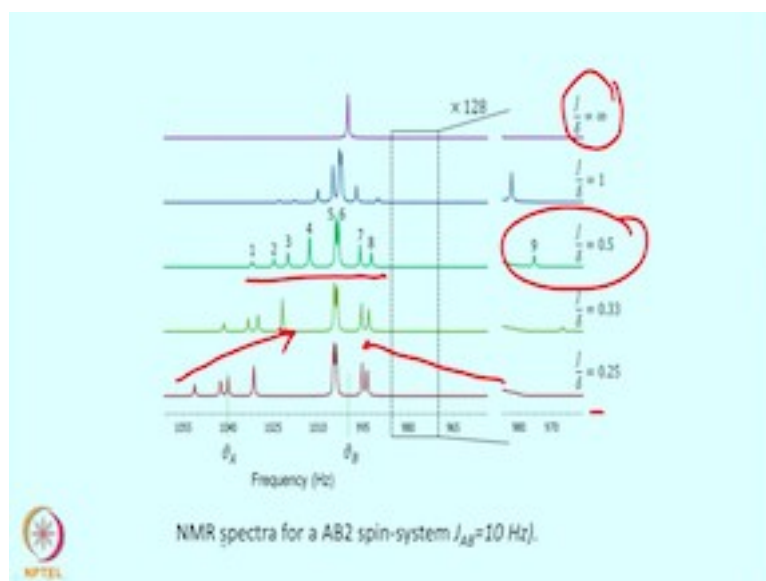
So we can derive energy for all these state and then one can start looking at what we get this spectrum so if you do rigorous analysis we get spectrum for AB_2 system like this so if the $\frac{J}{\delta}=\infty$, then we get actually one peak as we say is equivalent so this will be identical spins but as we start moving what we are seeing is that splitting pattern changes and if we have something like $\frac{J}{\delta}=0.5$, we have like 9 lines here.

And as we move here we can get even more splitting pattern like this so here one thing if you notice that we were discussing the spectral intensity are like this and this is called roof effect in the in the chemical shift. So because of the strong coupling this roof effect appears because of weak coupling as we saw in the last slide all are of equal intensity. So that is the A to B system and this we have simulated for AB spin system where we consider J_{AB} the coupling constant between A and B to be 10 hertz.
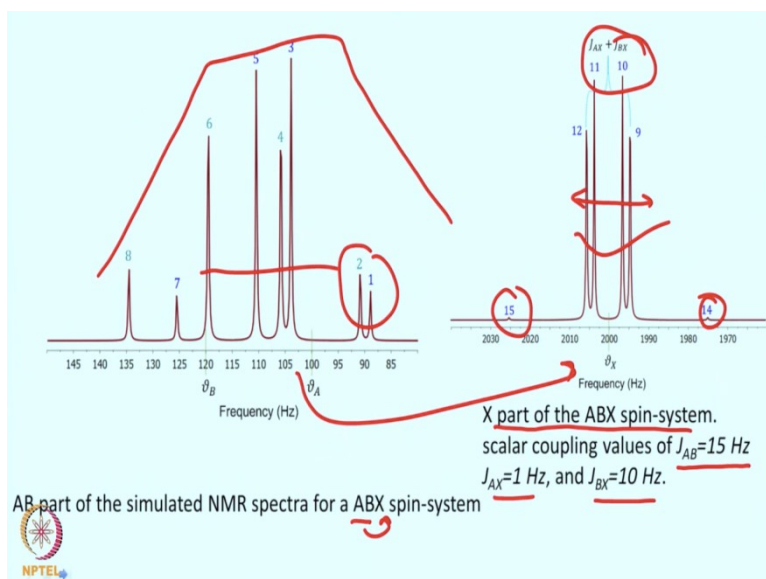
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Eigenvalues and Eigenfunctions in an ABX system

S.No	Eigen function	Energy
1	$\alpha\alpha\alpha$	$\frac{1}{2}(\nu_A + \nu_B + \nu_X) + \frac{1}{4}(J_{AB} + J_{BX} + J_{AX})$
2	$\alpha\alpha\beta$	$\frac{1}{2}(\nu_A + \nu_B - \nu_X) + \frac{1}{4}(J_{AB} - J_{BX} - J_{AX})$
3	$\cos\varphi_+(\alpha\beta\alpha) + \sin\varphi_+(\beta\alpha\alpha)$	$\frac{1}{2}\nu_X - \frac{1}{4}J_{AB} + D_+$
4	$-\sin\varphi_+(\alpha\beta\alpha) + \cos\varphi_+(\beta\alpha\alpha)$	$\frac{1}{2}\nu_X - \frac{1}{4}J_{AB} - D_+$
5	$\cos\varphi_-(\alpha\beta\beta) + \sin\varphi_-(\beta\alpha\beta)$	$-\frac{1}{2}\nu_X - \frac{1}{4}J_{AB} + D_-$
6	$-\sin\varphi_-(\alpha\beta\beta) + \cos\varphi_-(\beta\alpha\beta)$	$-\frac{1}{2}\nu_X - \frac{1}{4}J_{AB} - D_-$
7	$\beta\beta\alpha$	$\frac{1}{2}(-\nu_A - \nu_B + \nu_X) + \frac{1}{4}(J_{AB} - J_{BX} - J_{AX})$
8	$\beta\beta\beta$	$\frac{1}{2}(-\nu_A - \nu_B - \nu_X) + \frac{1}{4}(J_{AB} + J_{BX} + J_{AX})$

So that was *AB* system, next we can look at the *ABX* system, *ABX* means *A* and *B* are strongly coupled but they are weakly coupled to *X* so one can write the energy function for each of these states $\alpha\alpha$, $\alpha\alpha\beta$ so what I mean by $\alpha\alpha\alpha$ is something like this and $\alpha\alpha\beta$ something like this and as you go down $\beta\beta\beta$ is like this, $\beta\beta\alpha$ is like this and intermediates all they are mixed states because of the coupling constant.

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AB part of the simulated NMR spectra for a ABX spin-system

X part of the ABX spin-system. scalar coupling values of J_{AB}=15 Hz J_{AX}=1 Hz, and J_{BX}=10 Hz.

So in that case we have the spectrum that will come out to be something like this so here one can see because of *AB* strong coupled system we have again splitting pattern as we discussed earlier, it will have this roof effect of various transition, transition 1,

2, 3, 4 ,5 ,6 ,7, 8 and now here they are weakly coupled to X ,so they will split X and if you look at here because of $J_{AX} + J_{BX}$ this gives another four lines and these two very small lines here but one can see here intensity are more or less equal but there will be some effect.

So X part of ABX system comes like this and AB part comes like this. So here we have assumed that AB coupling constant is 15 hertz, AX is 1 hertz that and BX is 10 hertz. So that how spectrum will look like for a strongly coupled at AB and they are weakly coupled to X system.

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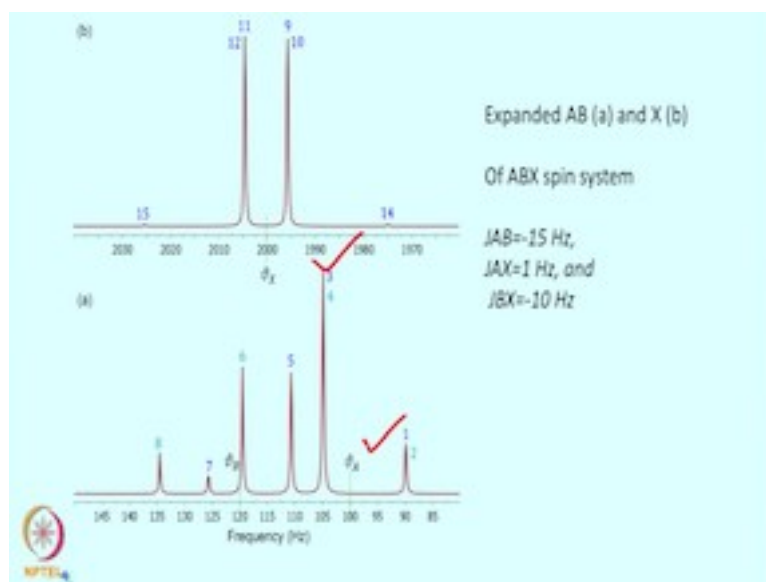
So one can expand and one can find it out this different spectrum for X spin and also for X spin and also for AB spins. So this is the kind of a spectrum for you can one can get it for strongly coupled AB system that are weakly coupled to B spectrum. So these are some of the rigorous analysis and as we look at that these spectra when they are strongly coupled they are not easy to interpret.

So what one trick one can apply that these are strongly coupled system and the coupling constant remains same so one option is to take these molecules and start recording spectrum at the higher field now chemical shift separation between them can increase and may be somewhat will convert to maybe weak coupling system and then one can start analyzing the spectrum.

So today I am going to stop it here and in the next class we will try to go little more detail, look at the effect of these couplings on the dynamic process or the chemical exchange process and we can build up the concepts from here. So thank you very much and looking forward to help you in the next class.