Advanced NMR Techniques in Solution and Solid – State
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Module-20
Receiver Phase and Phase Cycling
Lecture - 20

Welcome all of you, once again. In the last class we started discussing about pulse phase where I introduced what is the 90 degree pulse what is the phase of a pulse, first of all. What is meant by a 0 degree for pulse, what is the 90 degree phase pulse, what is 180 pulse phase, 270 pulse phase, etc. And we also discussed about what happened with the 90 degree pulse how it tilts the magnetization, the right hand thumb rule and then after tilting the magnetization by 90 degree pulse how it rotates.

For example, if I apply 90 degree plus X pulse what happens, if apply 90 degree – X plus what happens? And continuously we can apply 90, 180, 270, 360, like that, and make the magnetization to rotate in a direction perpendicular to the axis in which you apply the RF pulse. That is what we discussed, we applied pulse plus X on the plus X axis. And we saw that magnetization rotates in the YZ plane.

And depending upon whether you are going to apply along the X axis or - X axis, this rotation can be either clockwise or anti clockwise. That was about X axis, a rotation about X axis. That is what we discussed. So, we will continue further today and see what will happen for the rotation about Y axis. And then afterwards subsequently, we are going to what is the receiver phase, how to understand the receiver phase. So, we will start with what is called the rotation about Y axis today.

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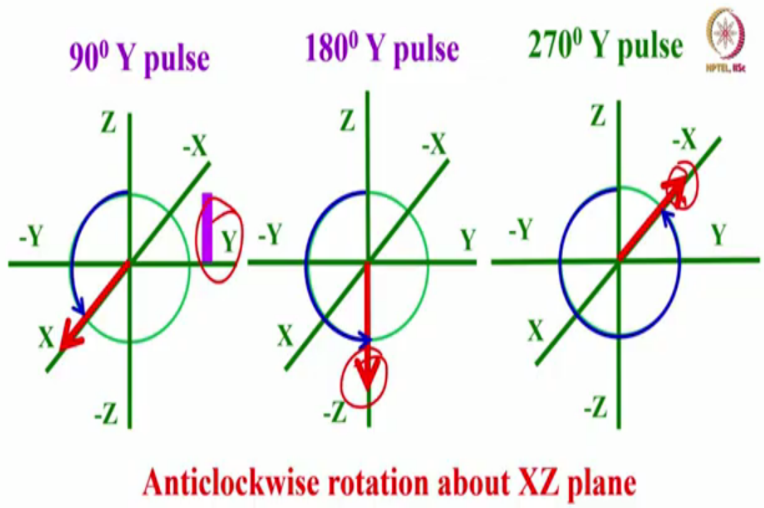

Now, I am going to apply a 90 degree Y pulse; start with the magnetization which is in equilibrium; which is in equilibrium, I apply 90 pulse which is along +Y; the magnetization if you apply right hand thumb rule, if it is like this, and then it will tilt back to Z axis, it is like Y axis. Now the curly fingers is telling me the direction of tilting, it tilts to plus X axis. So, this is a 90 degree pulse. So, now continue applying this, increase the length of the pulse in such a way the magnetization tilts to 180 degree to -Z axis.

Now continue and make the magnetization move to 270 degrees it comes to -X axis and then finally, you apply 360 degree pulse and bring the magnetization back to Z axis.

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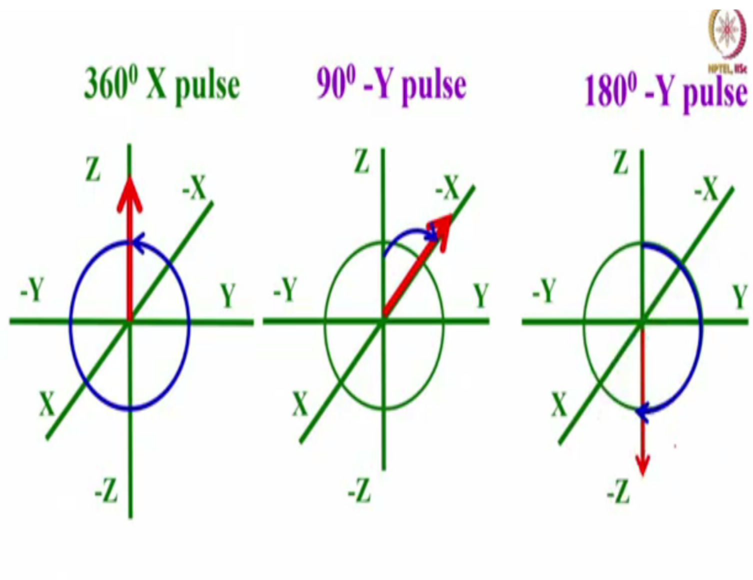

So, this is what happens, this is a clockwise rotation. So, we keep rotating from here, if you see from the center of this, you can see the rotation of the magnetization. So, now, we can also apply the same thing apply 90 degree -Y pulse instead of along plus axis, you apply along -Y axis. See what happens? the magnetization rotates in the opposite direction, you take it –Y, -X axis and then continue further; 180 will take it to, -Z.

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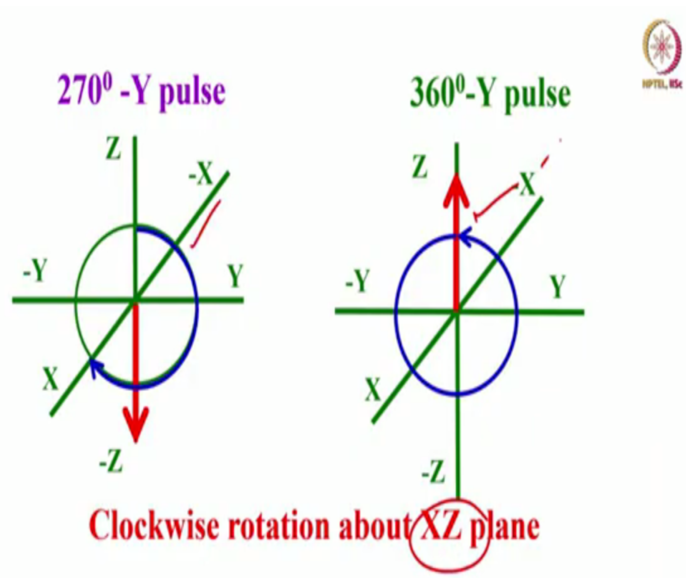

And then further 270 will take it to +X and then 360 again brings it back to Z axis. Again one complete rotation of the magnetization you can do. So, what have we understood so far. You can have the amplitude and power of the pulse; the width and power of the pulse you can tune it in such a way, you can apply the pulse either along the X axis or -X axis +Y or -Y axis. And tilt the magnetization to any angle you want. It need not be 90, 180 can be any, in between also.

So finally, you can make the magnetization to rotate in a direction in which you are applying the RF pulse, you can make it rotate clockwise or you can make it rotate anti clockwise; both are possible. So, this is where the phases of the pulses are very, very important. And with this, you can control the behaviour of the spins. You can tune the magnetization and design the pulses in such a way you can do whatever you want.

And make sure that the spins are rotated in a particular direction or in the particular plane so that you can get the information; retrieve the information from the spectrum, the way you want by designing pulses. So, pulse phase is very, very important. So, now this is a clockwise rotation of the YZ plane. Now completely we understood what is the rotation about the X axis? About Y axis, when you apply RF pulses and how the magnetization rotates.

Now I am going to introduce another thing called a receiver phase, you are applying the pulses along X or Y axis; that is a pulse phase. You can also have the receiver phase; you can see when they receive the signal how you receive?

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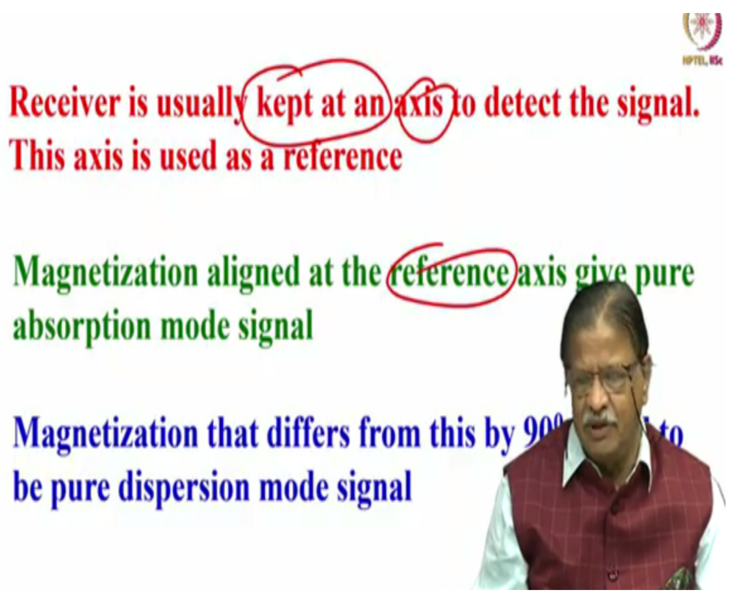

For example, receiver is usually kept at an axis to detect the signal; of course this should be possible even with the first class we told you, a magnetization is along Z axis, you apply a pulse on the X axis, you will have a receiver along Y axis to detect. So, they are all orthogonal to each other; all the three. The directions of application of the pulse, thermal equilibrium magnetization, and the detection, the receiver you are going to keep, all the 3 orthogonal to each other.

The way you tilt it depends upon where you apply pulse, that is ok. So, that is usually receiver is kept at an axis in the transverse plane. And this axis is called a reference axis that is important thing. The magnetization aligned along the reference axis gives you an absorption mode signal. Very important point, if I have a receiver in the axis where the magnetization is aligned, then I am going to get absorption mode signal.

If the magnetization differs by 90 degree from this, you are going to get it dispersion mode signal. This is a concept which we use very often now; the absorption mode signal, dispersion mode signal etcetera in understanding phase cycling.

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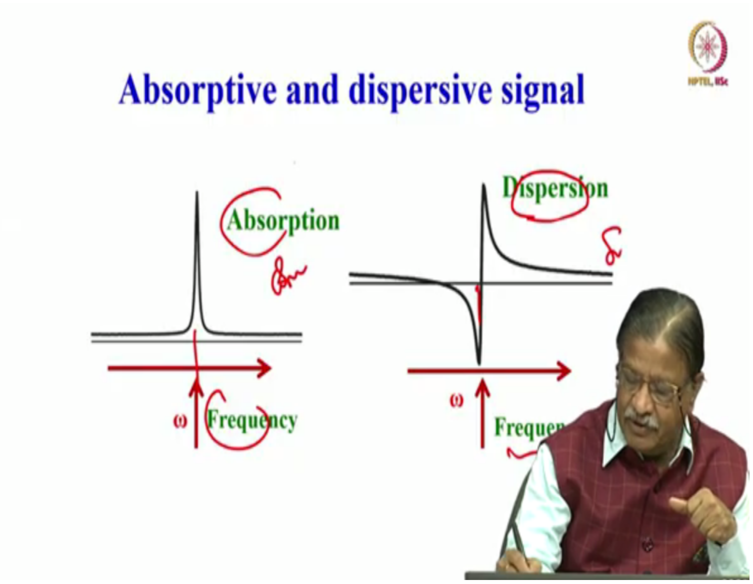

So, what is the absorption mode signal, what is dispersing mode signal? This is the absorption mode signal where you can see the signal positive and it is completely absorbed this is center of the peak and it gives the frequency of it. And this is in general called as an absorption mode signal. Same thing if the 90 degree out of phase, is the dispersion mode signal, it will be like this. Again at the center of this, this is where you can measure the frequency.

Absorption and dispersion are just out of phase by 90 degrees. Of course, when you were understanding the Fourier transformation, we knew that, this is a cosine part of the signal, this is the sin part of the signal we knew that; but anyway, I did not introduce that, but I am just telling you what is an absorption mode signal, what is the dispersion mode signal.

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You ask me a question what happens if I bring the magnetization to any other angle, at any other angle instead of being at X axis or Y axis. I have a receiver put just in between, let us say X and Z, axis somewhere at 45 degrees. What is the type of signal I get? It is neither absorption nor dispersion; it is the mixed phase; it has both absorption and dispersion character. If I apply a pulse, I have let us say this is my receiver phase, I have kept a receiver here and instead of tilted here exactly I tilt here, I am going to get absorption mode signal and the magnetization here will be dispersive mode; if I have a signal here somewhere in between, then you have component of the cosine component, and the sine component; both will be present. And that means, as a consequence of that, they are not exactly out of phase by 90 degree, the mixture phase will be present.

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So, another thing which we also discussed; the Fourier transformation. We knew the Fourier transformation gives both the real part and the imaginary component. I take a signal like cosine, sin or cosine are for the example, Gaussian or Lorentzian any function you take. And when we understood the mathematics of the Fourier transformation we knew that for the transformation of any function like that always results in real component and imaginary component; they differ 90 degrees. This is important point.

And the real part is what is called the absorption. That is what I said in the previous slide. And I see a signal like this which is absorption, when I see a signal like this, it is dispersive. This is the absorption signal, which is the real part of it. And dispersive is the imaginary part of it; or in other words this is the cosine part and this is the sin part of the Fourier transform signal.

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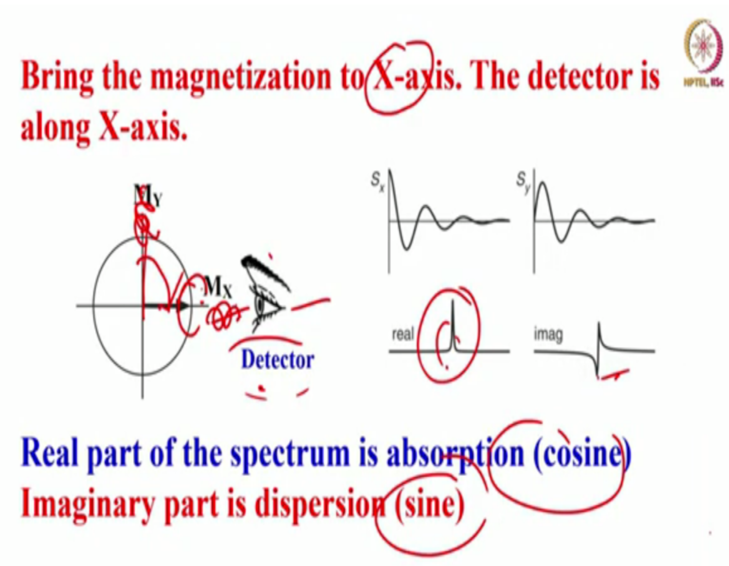

So, now, let us understand bit more. I will bring the magnetization to the X axis by applying 90 degree pulse. I will put my detector on the X axis, this what it is, I bring the magnetization from thermal equilibrium to X axis, it is my detector; I am detecting here, this is my receiver, detector means receiver I am telling, I am receiving the signal here. What is happening here? My receiver is here, magnetization is also on the same axis; what I should get? I told you? You must get an absorptive mode signal.

This is absorptive mode signal, because the Fourier transformation has a real and imaginary part. Now, the real part is absorptive this is here; and the imaginary part is out of phase by 90. There is a signal here; you have 2 receivers to receive, here one receiver receives this and the other receiver receives this signal. Then what will happen? that will be signal along MY; the MX and MY components of the magnetization will be there. MX component, will be detected as a pure absorptive mode, where as MY component will be imaginary part. It will be out of phase by 90 degree, it is a dispersive component.

So, that is simple; you are applying 90 degree pulse bring the magnetization into X axis, My detector is along the X axis; absorption is real and dispersive is imaginary; and then MX component is absorption and MY component is imaginary. So, the real part of the spectrum is always for the cosine and imaginary part is always dispersion part and is the sine component.

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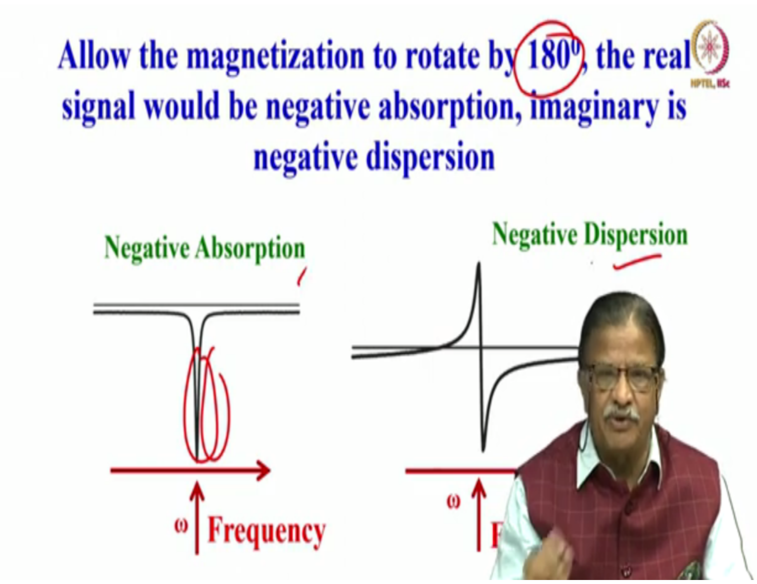

Now, what I will do is after bringing the magnetization here, I will allow it to process, that is rotate by 180 degree then what will happen? The signal will start coming here; magnetization moves here; from plus axis it moves to -X axis then what is going to happen? if the signal move by 180 degree, then real part will become negative absorption; whereas the dispersive part becomes negative dispersion. Again it is out of phase by 90 degree. So, what is going to happen the real part will be negative absorption and imaginary part is negative dispersion, when I allowed the magnetization to rotate by 180 degrees.

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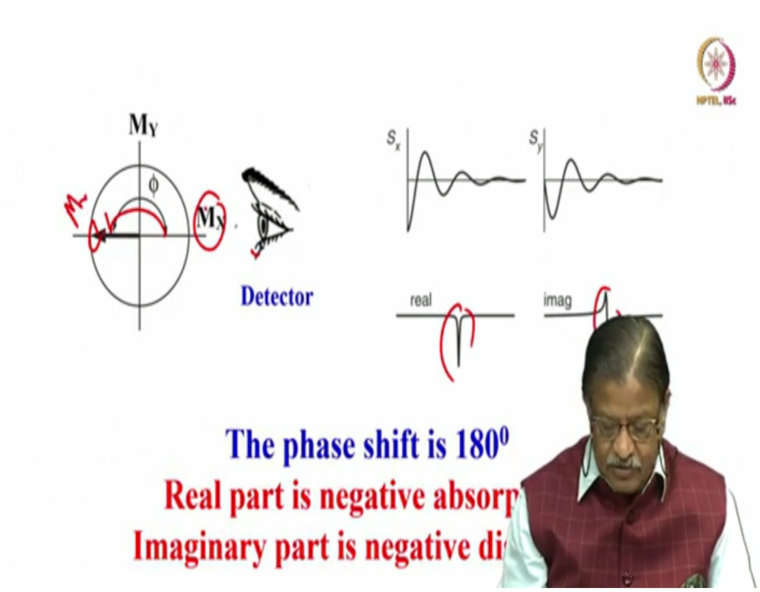

Now, what I am going to do is, this is what the signal what we observed this the negative absorption. This is imaginary part, now, I have moved the magnetization from this to this; either way, whether you move clockwise or anti clockwise does not matter, they have rotated. Now, once MX signal is here, and now I am detecting signal here. So, what we are going to get is negative dispersion, in fact MX I should put here, because it is already moved here. So, the phase shift is 180 degree. So, real part is negative absorption and imaginary part is negative dispersion; fine.

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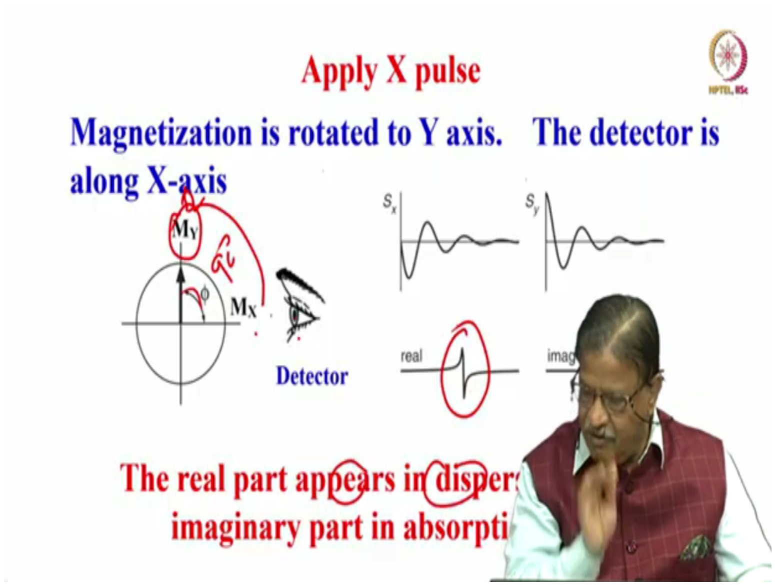

Now, I would apply X pulse and rotate the magnetization to Y axis; the detector is along the X axis; this is what we are going to get. Now, remember, I am applying the X pulse, the magnetization is along Y axis, on Y axis; but my detector is still here, receiver I have not changed. So, what is going to happen? there is the phase shift already be 90 degree what does it mean? The real part now becomes like a dispersive signal.

And imaginary part becomes like a absorption signal; it looks like absorptive because both of them are changing in the phase by 90 degree. But I have not changed the position of my receiver, my receiver is here only, but the magnetization is out of phase by 90 degree. So, the real component of it is dispersive, looks like dispersive; whereas, the imaginary part looks like absorptive. So, this is the important point when you apply pulse on the X axis and still your receiver is not changed.

So, what do you understand from this? You can apply pulses in any axes, and you can also change the axis of the receiver, receiver need not be here. On the other hand, if I move the receiver here what would have happened? still you would have got absorptive the signal in the real part and dispersive in the imaginary if the receiver has moved here, while I move the magnetization 90 degree. I can also move the receiver in the same direction; along with the MY I will also move on 90 degree. Then you are going to get absorptive. And this will be imaginary, but right now, our magnetization is here and our detector is here this is what the signal.

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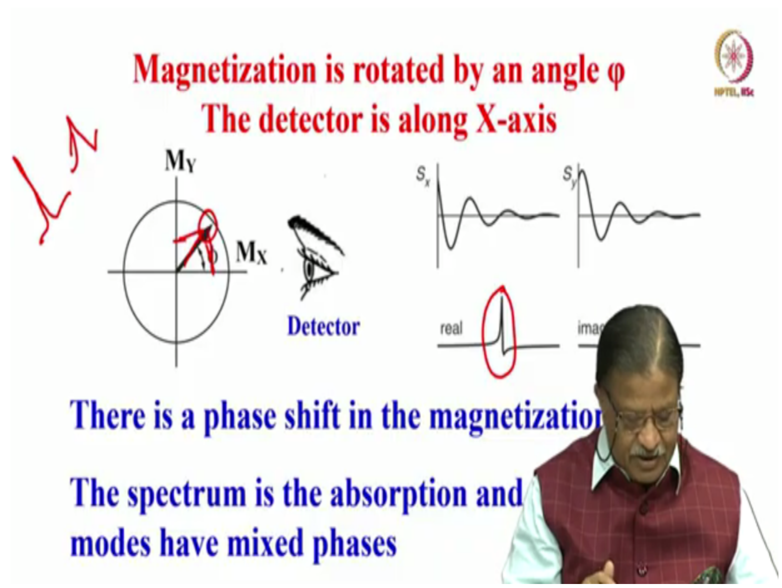

Now allow the magnetization rotate by any angle phi; as I told you it is somewhere here; what is the signal you are going to get? Now, you have a MX component as a MY component both are present here; MX and MY both are present. So, it is a mixture of absorptive and dispersive; see here it is not absorptive, there is a phase error here, phases if it is really pure signal there should not be any phase error; it should be like this, here there is phase error like this signal.

So, there is a mixture of phase here; it is not pure absorptive not pure dispersive. Similarly, in the imaginary part also, there is a phase distortion this is a mixed phase. So, this is what happens when you apply the pulse at any other angle other than the 90 degree; you will have a mixture of components from real and imaginary. The phase is not pure phase, it is the mixed phase.

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So, now, you may ask me a question I need to detect both the signals. How do we do that? Of course, in NMR that is what is done, we detect both the real and imaginary part of the signal. That means we have 2 receivers that are kept out of phases by 90 degree; this is called quadrature detection. I told you in earlier course, what is the quadratic quadrature detection.

I have 2 receivers kept exactly out of phase by 90 degree. One receiver R1 here other is R2 here, receiver 1, receiver 2; then here I will receive real part; in this receiver I will receive imaginary part of the signal. Both I can detect, that is, 2 receivers are required. So, in quadrature detection generally we do that and they should be exactly out of phase by 90 degree, otherwise there will be phase error and we need to correct the phase. And remember how do we correct the phase, we discussed this when we discussed the Fourier transformation.

Now, I will introduce something about Fourier transformation of a cosine and sine function, because we require this for understanding the phase cycling. You know what is it cosine function?

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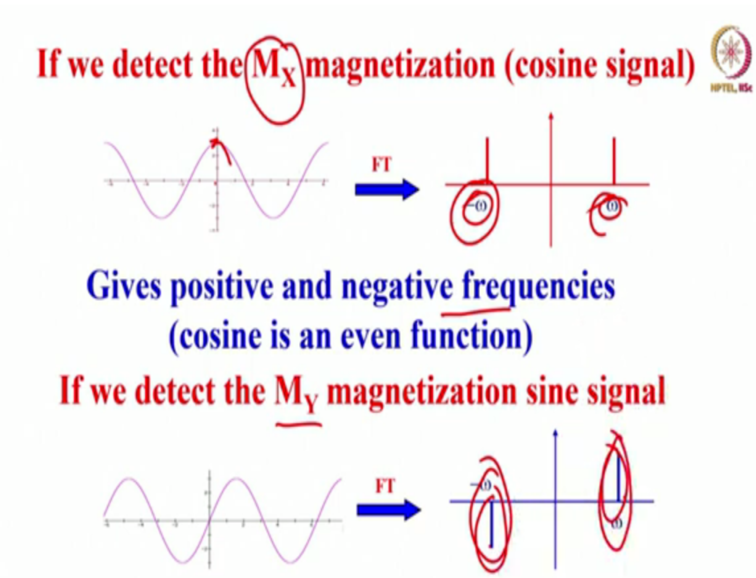

Cosine function is very simple. The detected signal MX with the receiver is also along the X axis is a cosine signal. And you start like this, it is like this starts with X at 0 the maximum value is 1 and it is oscillatory function, this is cosine function. Now, I do the Fourier transformation of this; I get 2 frequencies real and imaginary which are plus omega, minus omega. This is the Fourier transformation as a cosine function gives negative and positive frequency, why negative and positive frequency? because cosine is an even function. Now, if you detect MY magnetization, it is a sine signal. Of course, this is the MX magnetization, I am talking, we get 2 signals. Now if MY magnetization if I detect that is the sine part or of course, this itself cosine signal itself; you do this thing, then Fourier transformation of this you get minus omega and plus omega they are out of phase by 90 degree; one is negative absorption, and the other is positive absorption.

See, if you detect the MX part of the signal and do the Fourier transformation of it, you get 2 frequencies minus omega and plus omega, because the cosine is an even function, if you detect this MY component of it, that is the sine component. When you do the Fourier transformation you get again 2 frequencies minus omega and plus omega, omega is a frequency. But one is negative omega is negative absorption peak, positive omega is positive absorption peak. This is what you are going to get; the Fourier transformation of sine function is the Fourier transformation of the cosine function.

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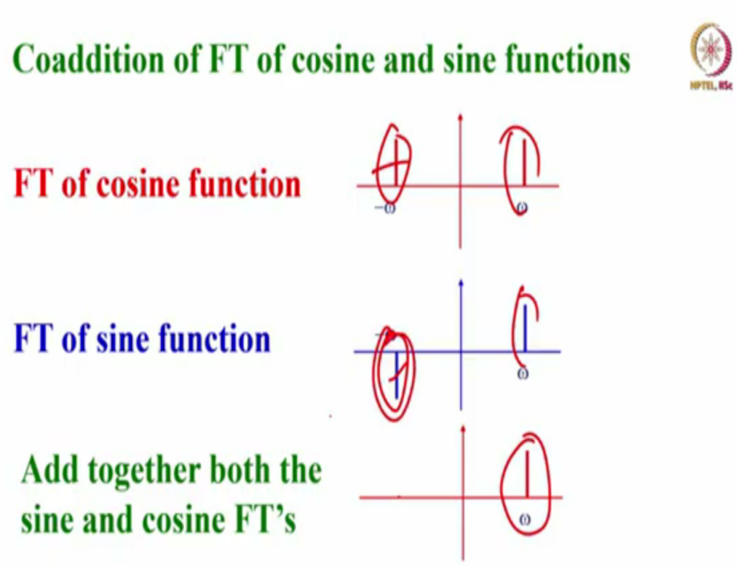

Now I will do on trick I will do the Fourier transformation of both these functions individually, this is the FT of the cosine function that is what we discussed, we have negative and positive absorption. I will take the FT of cosine function. I have negative and positive both are there. Let me add up both of them; what will happen? if add both Fourier transformations together. Fourier transformation is a linear function, I told you; we can also add it up with the time domain or in the frequency domain; you add up both of them. Then what will happen? this will cancel out positive or negative signal; and we are going to get only one signal which is at plus omega. This is what we do. We will do this very often; I can eliminate one of the components; imaginary component now, siine component or the negative component I removed, I get only positive signal bythe coaddition of the Fourier Transformation of cosine function and the sine function.

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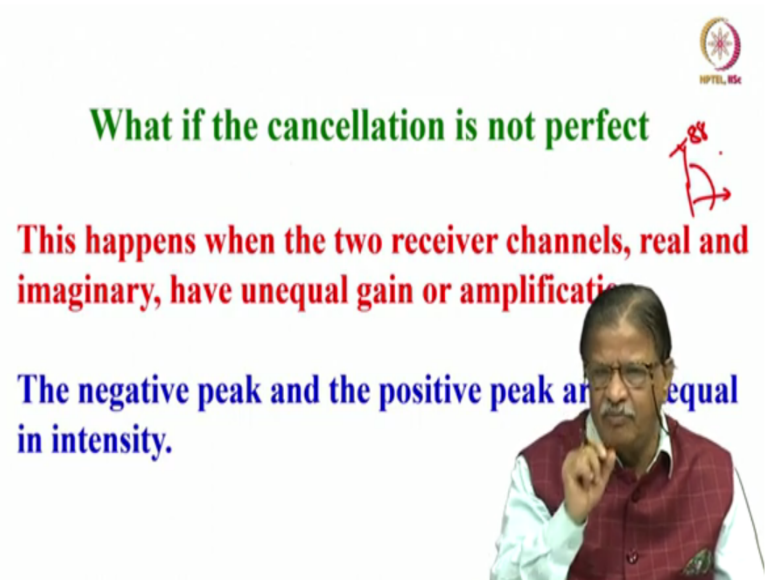

Now, you ask me a question, what is going to happen if the cancellation is not perfect, that is what I told you. The real and imaginary part the detectors should be exactly out of phase by 90 degrees. In the electronics, in the equipment the gain should be equal, if the gain is not same or exactly they are not out of phase by 90 degree, there will be a phase error. Even though you have a detector at exactly 2 places like this. Let us say the phase difference is not 90, it is about 88 you get into phase errors.

Now, this happens for unequal gain or amplification. Negative and positive peaks are not of equal in intensity. Then what will happen? There is no cancellation at all, cancellation is not efficient. I do the Fourier transformation of the MX component, get negative omega and positive omega. I take the Fourier transformation of the MY component, take negative omega and positive omega; negative omega here is negative dispersion I will co-add it. But instead of cancelation there will be some portion of the signal left there. It is not going to completely cancel out.

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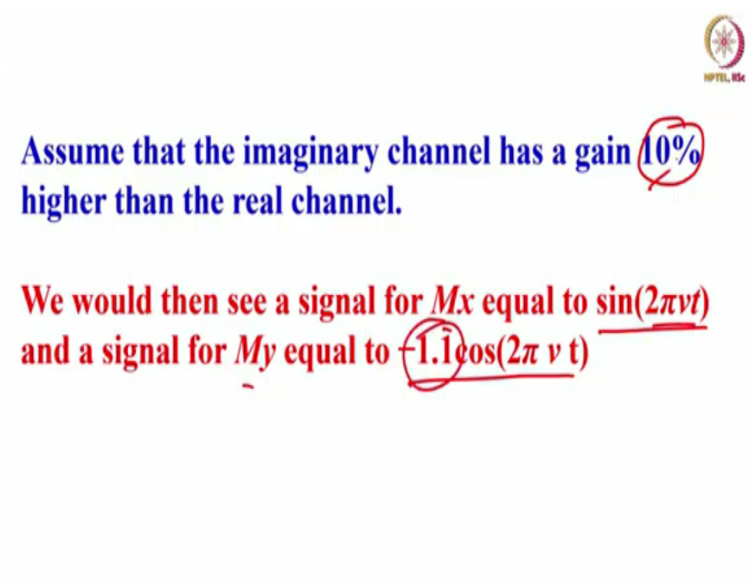

Then what will happen? It gives raise to the problems; what do you do in such a situation? This is where receiver phase, pulse phase understanding is very, very important. We can do some trick to cancel it. Let us assume the imaginary part has a gain of 10% more than the real signal. See, I will do it for a transformation the real part is let us say cosine part is 10% more than the sine part. So, cancellation is not a possible here, 100%.

Now, you see a signal MX equal to sine some frequency, a signal for MY = cosine of 2 pi nu into t; true. Because what is going to happen is this is not 100% equal. So, this is 2 pi nu t. This is 1.1 times because 10% more I have taken as the gain; imaginary part is 10% more.

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Carry out four acquisitions, each time change the pulse phase

Scans	Pulse Phase	Magnetization vector starts at	M_X	M_Y
1	+X	-Y	$\sin(2\pi\nu t)$	$-1.1\cos(2\pi\nu t)$
2	+Y	+X	$\cos(2\pi\nu t)$	$1.1\sin(2\pi\nu t)$
3	-X	+Y	$-\sin(2\pi\nu t)$	$1.1\cos(2\pi\nu t)$
4	-Y	-x	$-\cos(2\pi\nu t)$	$-1.1\sin(2\pi\nu t)$

$$\text{FID (Real)} = Mx(1) + My(2) - Mx(3) - My(4) = 4.2\sin(2\pi\nu t)$$

$$\text{FID (Imag)} = My(1) - Mx(2) - My(3) + Mx(4) = -4.2\cos(2\pi\nu t)$$

So, now we carry out 4 acquisitions; 4 experiments, which means I will acquire the signal 4 times. And each time I do a trick, I will change the pulse phase. First time, I will do an experiment collect the signal, first experiment; I put my pulse phase along +X, that is I put the RF pulse along +X axis. Then magnetization as you know, when I apply 90 degree pulse, does not matter whatever the gain, phase difference between 2 receivers, My pulse is along the X axis it is the 90 degree pulse.

It has to bring the magnetization to –Y that I know; it will bring the magnetization to –Y. Now, MX component will be sine of this, and the MY component 1.1 cosine of this one. That is correct, because we have seen that. Now I will do another experiment, I put the pulse along +Y, the magnetization comes around +X. And then again, this cosine part will be MX and sin part will be 1.1 times MY. It is simple that is what we understood so far. When you apply RF pulses at different axes, where does the magnetization come. And if you have a receiver at different axis; how we get the MX and MY components, we discussed. We now do a third experiment, apply a RF pulse along -X, the pulse phase is –X and receiver phase is +Y, then this is what the signal you are going to get for MX and MY. Do a fourth experiment at -Y, the signal starts at -X and you are going to get the MX as cosine part and MY as the sine part like this, fine.

See, somehow the 10% gain of the imaginary part is like this, because I am changing the receiver every time at different places; now, you see once it is -1.1 times cosine of this ,you see; 1.1 time sine, 1.1 time cosine, - 1.1 of one time of sine function. What is the FID of the real part, it is the Mx of 1, this is; one +My of 2, this one; -Mx of 3 and –My of 4. All the 4 is nothing but the FID ofe the real part. I add up all these things then I am going to get 4.2 times sin of 2 pi nu t.

So, in another case what I will do, I will take the FID of the imaginary part, that is, this is whatever you took Mx, you have to take My for this now, the imaginary part. My of 1 you take and Mx of 2 or My of 3 and Mx of 4 you take. And now co-add everything. It turns out to be -4.2 cosine of 2 pi nu t. What did you do? Now, although gains of the these 2 receivers may not be exactly out of phase by 90 degree, when you do the phasing of the pulses and also the receiver in such a way to change the position of the pulses and change the position of the receiver; when you do 4 different experiments and coadd the signal; this is also +4.2 times it is -4.2 times. Now whatever what you have done. The 2 FIDs are the perfectly balanced.

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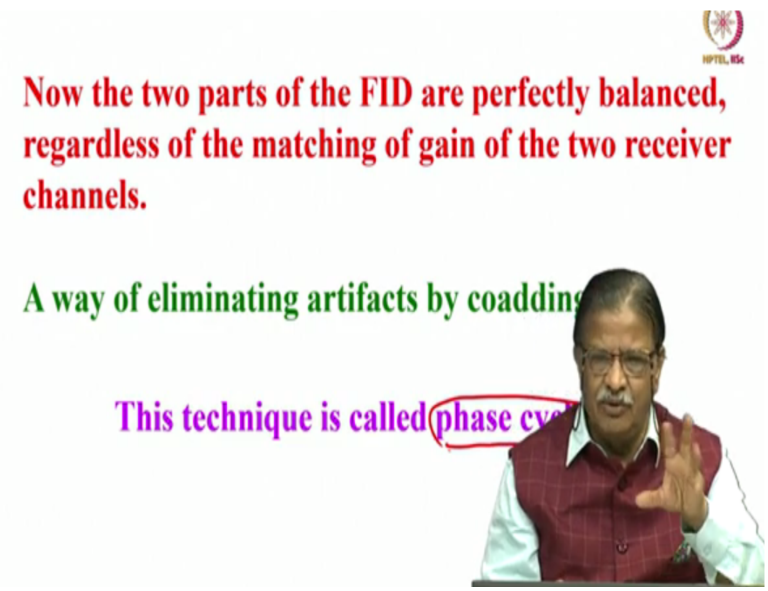

2 parts of the FID, the real part and imaginary part are perfectly balanced, does not matter whether the 2 receivers were matching or not, the gain may be different, but as far as we are concerned, when we start collecting the signal we have managed in such a way that both real part of the signal and imaginary part of the signal get completely balanced.

Now, what will happen? what did we achieve? this is what is called the elimination of the artifacts. This is an instrumental artifact, because the gain is not exactly same. By doing this type of experiment by coadding the signal, we have removed the artifact which comes because of imbalance in the receiver gains; which is not balanced. What do you call this technique? This technique is called phase cycling. Phase cycling is a method in NMR, where you can cycle the phase of the receiver; or you can cycle the phase of the pulses, either of them you can do; design the way you want to see that this type of artifact can be eliminated. Not only for this, you can also do this type of phase cycling to get particular information you want. I can get a particular signal; when we talk about coherent selection everything, I will discuss these things.

So, this way, the phase cycling component is very, very important in NMR. That is what I wanted to tell you, the receiver phase and the pulse phase must be very clear in your mind. Depending upon where I apply the pulse where I place the receiver, whether the detected signal is real or imaginary, whether it is absorptive or dispersive; or is a mixture, everything we know. And based on that we can manipulate in such a way, we can get the signal without any errors, without any phase artifacts, as it is coming because the instrument or because of collection of signal due to phase distortion.

So, all these things we can do; this is called phase cycling. So, this is what I wanted to tell you is about the receiver phase and the pulse phase. So, today, in the last class and this class, what we understood is how we can deal with the phases of the pulses. What is a pulse phase? How do we tilt the magnetization about different axis. Don't ever get confused at all; simply remember, pulse phase is the phase of the pulse, in which axis you are applying. If you apply a pulse along the X axis, it is the 90 pulse means 90 X pulse, if you are applying along Y axis is it is 90 pulse means 90Y; similarly 90 – X is 90 – X; this is the pulse phase. Similarly, receiver phase where you keep the receiver, receiver that is on the X axis or Y axis or –X or -Y. Accordingly the detected signal is either absorptive component or dispersive component. Sometimes, it is depending upon whether receiver is here, whether the magnetization this is along the X axis magnetization is along Y axis, what are you going to get? You will get real part dispersive and imaginary part absorptive. So, this is what happens. So, all these things if you understand, you can start playing with these pulse sequences; playing with pulse phases and receiver phases and design the pulse sequence of our choice. Orchestrated way we can get the information we want from the NMR spectrum. So, this is what I wanted to tell you about this today. So, now time is almost coming to an end I am going to stop now. In the next class we will talk about evolution of chemical shifts and evolution of the J coupling in different pulse sequences. There I am going to introduce this, now I introduce absorptive dispersive component, there I am going to introduce in phase and anti phase signal. How do you understand those things? And how the magnetization evolves, how the chemical shift evolves, how the coupling evolves when we acquire the signal in different pulses. This we will discuss in the next class. I want to stop here. Thank you.