NMR Spectroscopy for Chemist and Biologists

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Lecture No. 14

Theorems on Fourier Transform

So let us continue the discussion Fourier transform and NMR spectroscopy which we started in the last class. While we do so it is a good idea to have a recap on what was done last time in a brief manner.

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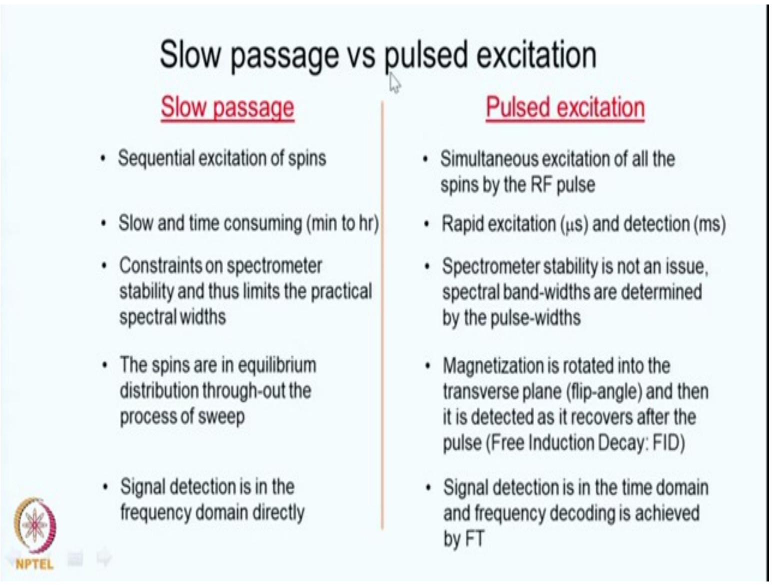

Slow passage vs pulsed excitation

Slow passage	Pulsed excitation
Sequential excitation of spins	Simultaneous excitation of all the spins by the RF pulse
Slow and time consuming (min to hr)	Rapid excitation (μs) and detection (ms)
Constraints on spectrometer stability and thus limits the practical spectral widths	Spectrometer stability is not an issue, spectral band-widths are determined by the pulse-widths
The spins are in equilibrium distribution through-out the process of sweep	Magnetization is rotated into the transverse plane (flip-angle) and then it is detected as it recovers after the pulse (Free Induction Decay: FID)
Signal detection is in the frequency domain directly	Signal detection is in the time domain and frequency decoding is achieved by FT

So therefore, I have here a general introduction and general coverage of what we did last time, slow passage verses pulsed excitation, this is an integral element of the Fourier transform NMR spectroscopy and this was the conventional method which was used before the discovery of the Fourier transform NMR.

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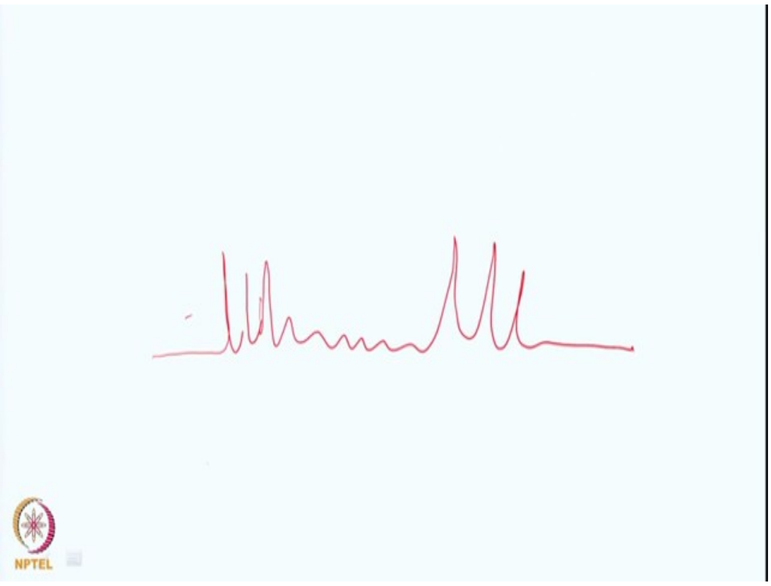

To give a recap of what this means let us just have a look at NMR spectrum once more, you have an NMR spectrum which looks generally like this with lots of signals at various places in the NMR spectrum.

Now we said in the slow passage experiment so once has to satisfy the resonance condition for each one of this and so therefore, when the resonance condition is satisfied for this peak you will see absorption signal there, when it is satisfied this peak you will see the absorption signal there and so on and so forth. We said this as to go on slowly because the system has to follow the magnetic field, when you change the magnetic field to satisfy resonance condition by one by one the system has to be in equilibrium all the time therefore, this passage has to be slow and we do a sequential excitation of the individual spins.

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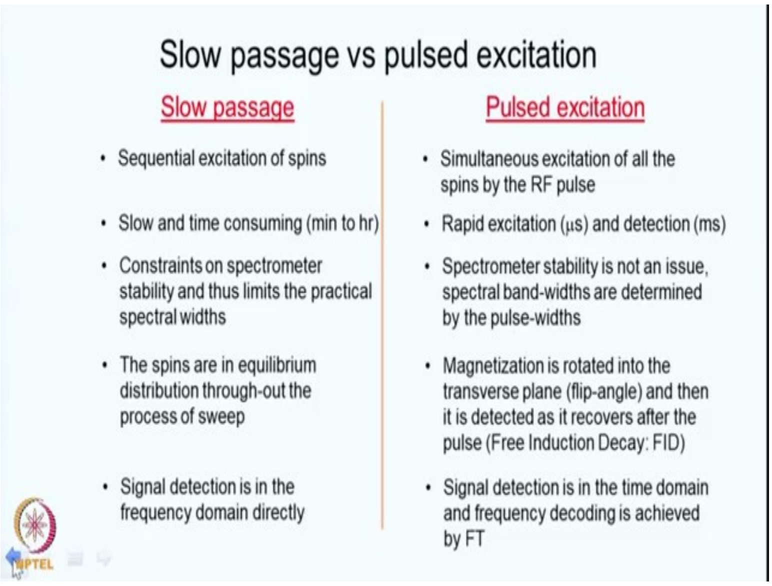


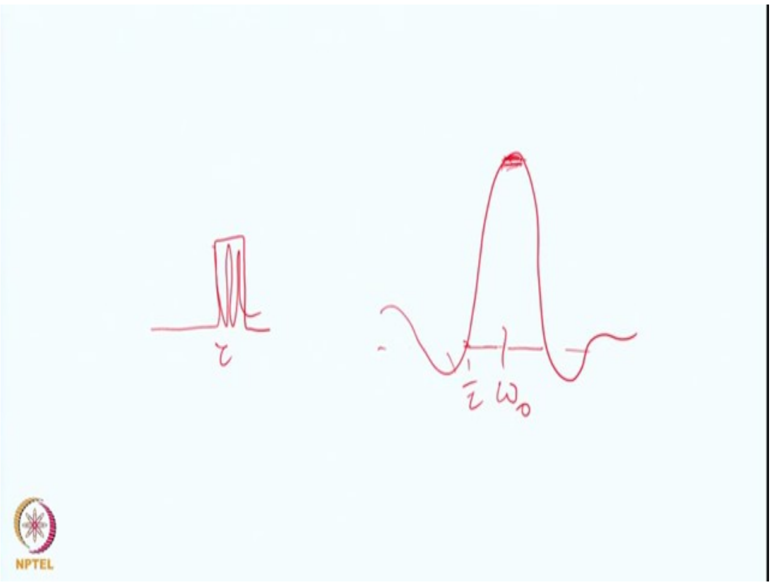
Slow passage vs pulsed excitation

Slow passage

- Sequential excitation of spins
- Slow and time consuming (min to hr)
- Constraints on spectrometer stability and thus limits the practical spectral widths
- The spins are in equilibrium distribution through-out the process of sweep
- Signal detection is in the frequency domain directly

Pulsed excitation

- Simultaneous excitation of all the spins by the RF pulse
- Rapid excitation (μs) and detection (ms)
- Spectrometer stability is not an issue, spectral band-widths are determined by the pulse-widths
- Magnetization is rotated into the transverse plane (flip-angle) and then it is detected as it recovers after the pulse (Free Induction Decay: FID)
- Signal detection is in the time domain and frequency decoding is achieved by FT



Sequential excitation of the spins is what is what is done in the slow passage experiments, whereas in the pulse excitation we apply an *RF* pulse the *RF* is applied for a short period of time and the response of this is generation of a large number of frequencies and therefore, we have a simultaneous excitation of all the spins by the *RF* pulse. The *RF* pulse is applied for the short time tau and then we also saw what is the response of that which is a kind of sink function and we have a certain bandwidth which is excited by the *RF* pulse.

Now this is a slow and time consuming process, this can take minutes to hours, whereas this is a rapid excitation the pulse is applied for a few microseconds and we detect the signals as free induction decay so and therefore, this is a much faster way of recording the NMR spectrum.

As a result of this we can do rapid signal averaging here and we will see more of that in the present today's class. And this slow experiment in a slow passage puts lots of constraints on spectrometer stability and thus limits the practical spectral widths. Because if we have scan through a 10 ppm range which is about 1000 Hertz in the case of proton for 100 megahertz spectrometer, we said it will take 15 to 16 hours.

And then if we have to signal average with large number of scans then it can take 1500, 1600 minutes that puts the heavy constraints on the spectrometer stability, it has to be stable producing the same kind of a magnetic field and there should be no fluctuations in the temperature around and things like that.

Therefore, this puts the serious limits on the practical numbers for the spectral widths, whereas here the spectrometer stability is not an issue because you are collecting the data in about a few milliseconds, spectral bandwidths are determined by the pulse widths, you remember we had the pulse widths which is typically of order of 5000 to 6000 Hertz and that can be readily exited and we when we apply the pulse like this which is here you have the *RF* going on a short period and the response of this was something like this.

So then, we had, this is the main frequency $\omega_0$of the RF and which this is the area which is quite substantial and this one is roughly approximately equal to $\frac{1}{\tau}$, so if the τ is the length of the pulse, if that is of the order of 1 microsecond, then here you have almost 1 Megahertz here, this range is 1 Megahertz, this range is 1 Megahertz therefore, a few Kilohertz here will have the uniform excitation efficiency and therefore, we are able to select these with the application of the *RF* pulse.

So therefore, excitation of all the spins which happens in few microseconds and we can collect the data quite rapidly. And in this case the spins are in equilibrium as I mentioned throughout the process of sweep. It follows the magnetic field and that is the reason why we had to do it slowly, in this case magnetization is rotated in transverse plane flip angle.

Notice that magnetization which is otherwise on the Z-axis when we applied the RF pulse it gets tilted into the *xy* plane. Therefore, we said we can apply a 90° pulse or a 180° pulse or a 270° pulse we described all of this things and 90° puts the magnetization in the transverse plane so also 270° pulse. But, we can apply any kind of flip angle it may not be of 90° it can be 20, 30, 40 whatever depending upon your choice and that discussion we can do later.

Now and then the signal is detected in the absence of the *RF* and therefore and it is called as a free induction decay because it is free precision in the absence of any perturbation the signal is induced in a detector is consist as a voltage because of precsing magnetization induced a voltage in your detector and that is your signal and the signal decays because of the relaxation behavior of the spins, transfers magnetization in the decays and therefore this whole signal is called as free induction decay.

Signal detection in the slow passage happens in the frequency domain directly, whereas in the pulse excitation signal detection is in the time domain and frequency decoding is achieved by Fourier transformation, we said all this signals are exited at the same time and the different magnetization components precess in the transverse plane as they precess they are all individually induced signal in the detectors. Therefore, what we will observe is the super position of all of these signals components from the various precessing magnetization. Therefore, this can be decoded by doing the process of Fourier transformation.

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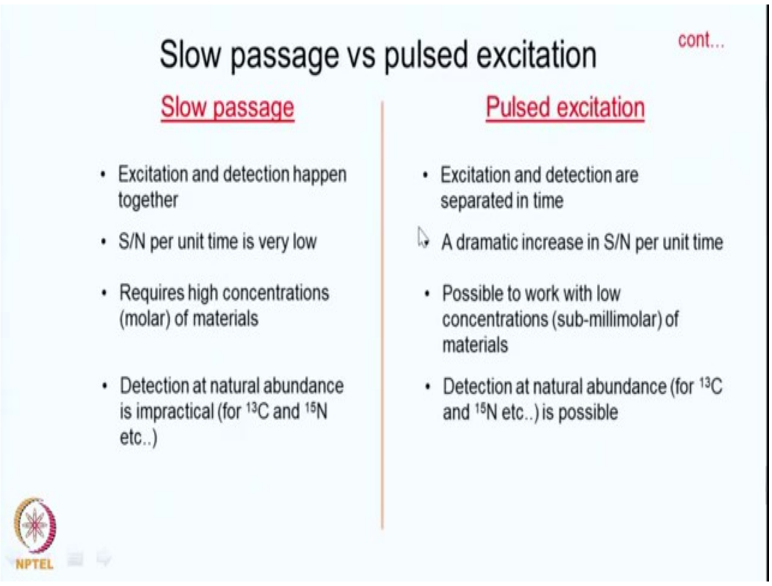

Slow passage vs pulsed excitation

cont...

Slow passage	Pulsed excitation
• Excitation and detection happen together	• Excitation and detection are separated in time
• S/N per unit time is very low	• A dramatic increase in S/N per unit time
• Requires high concentrations (molar) of materials	• Possible to work with low concentrations (sub-millimolar) of materials
• Detection at natural abundance is impractical (for ^{13}C and ^{15}N etc..)	• Detection at natural abundance (for ^{13}C and ^{15}N etc..) is possible

So a consequence of this is the following, excitation and detection are separated in time in pulse excitation, whereas, here excitation and detection happen together, what I mean excitation and detection are separated in time we apply an *RF* and following the *RF* we detect the signal as an FID.

So therefore, a signal averaging is much better here compared to this, here for one can it takes about 15 minutes for here one can it take about few milliseconds, few hundreds of milliseconds. Therefore, as a result of signal averaging you have better signal to noise ratio per unit time in this case as compared to what it is in the slow passage. This was an actually a major breakthrough and that led to the application of NMR to various kinds of systems.

So here one require very high concentration of materials molar concentrations, whereas here one code word with low concentration of materials sub millimolar materials, you may be often be limited by the solubility of the molecules in your solutions therefore, you can work with small concentration of materials you can do better signal averaging and get higher signal to noise ratio.

In the case of nuclei such as carbon 13 and nitrogen 15 and many others, which have very low natural abundance it would we almost impossible to detect signals by the slow passage experiments because this signal to noise will be very very low, remember C13 in 1.1 percent and nitrogen 15 is 0.37 percent, to collect signals from such kind of low abundant nuclei slow passage experiment would be almost impossible to perform. Whereas here you can do it because your signal averaging several times you can go at their FIDs and Fourier transform at the end. So this is the important differences between pulse excitation and Fourier transformed NMR and compares to the slow passage experiments.

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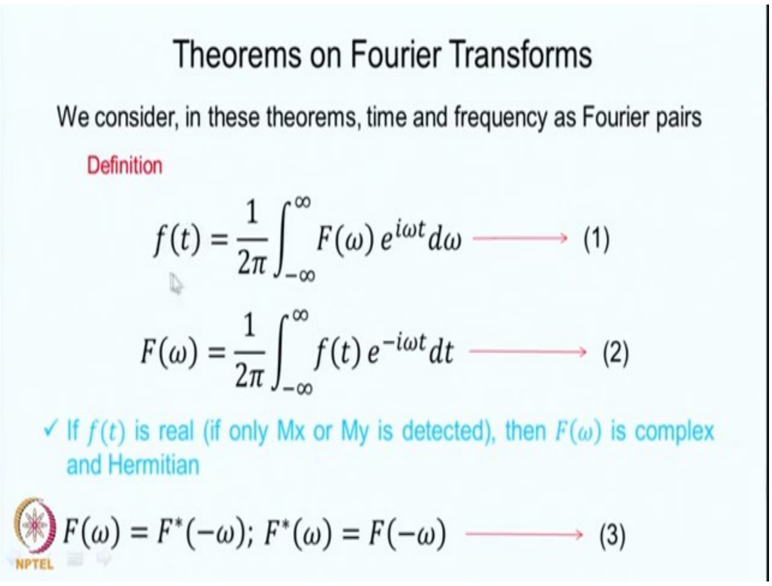

Theorems on Fourier Transforms

We consider, in these theorems, time and frequency as Fourier pairs

Definition

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)\, e^{i\omega t} d\omega \longrightarrow (1)$$

$$F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)\, e^{-i\omega t} dt \longrightarrow (2)$$

✓ If $f(t)$ is real (if only Mx or My is detected), then $F(\omega)$ is complex and Hermitian

$$F(\omega) = F^{*}(-\omega);\ F^{*}(\omega) = F(-\omega) \longrightarrow (3)$$

So now, we will go forward from here on and that is to make some formal definitions of the Fourier transformation. Some theorems on Fourier transforms is what we are our on to consider now. First of all the definition the Fourier transform definition, this is a mathematical operation

$$f(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{i\omega t}\,d\omega\,\ldots\ldots\ldots\ldots\ldots(1)$$

so this is the definition and this actually represents our FID, FID is the superposition of all frequencies precising in the transverse plane and that is mathematically represented in this manner.

Conversely you can write the frequency domain spectrum as the Fourier transform of the FID

$$F(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)e^{i\omega t}\,dt\,\ldots\ldots\ldots\ldots\ldots(2)$$

So this is the operation one performs, we consider the signal we collect the signal f of t as FID and they do your Fourier transformation in this manner and we get the frequency domain spectrum. Now, what are the properties of this functions and this will follow from this definitions without going to the actual detail calculations here we can list some of this properties, Ok.

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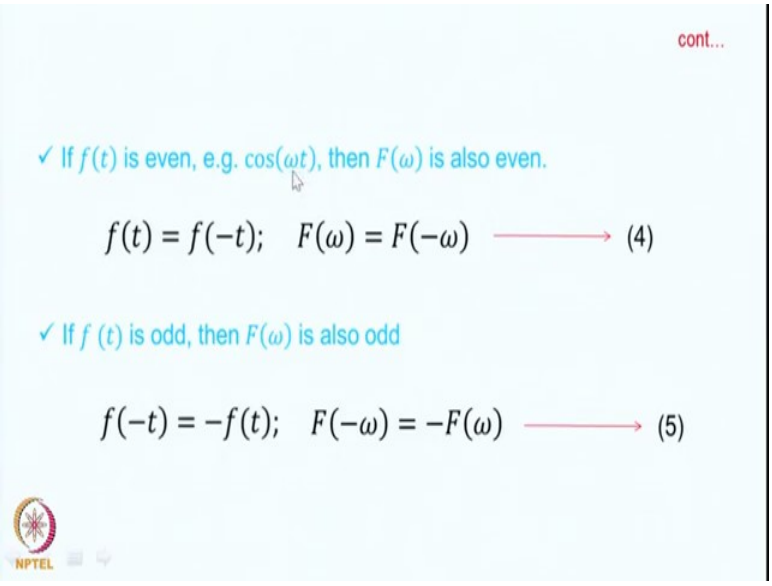

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- ✓ If $f(t)$ is even, e.g. $\cos(\omega t)$, then $F(\omega)$ is also even.

$$f(t) = f(-t); \quad F(\omega) = F(-\omega) \longrightarrow (4)$$

- ✓ If $f(t)$ is odd, then $F(\omega)$ is also odd

$$f(-t) = -f(t); \quad F(-\omega) = -F(\omega) \longrightarrow (5)$$

Now you can see f (t) is even, that is if the function is cos (ωt), cos (ωt) is even function. What does that mean? If we change t to minus t it still has the same value cos (ωt), and then F(ω¿ is also even.

$$f(t)=f(-t); F(\omega)=F(-\omega)$$

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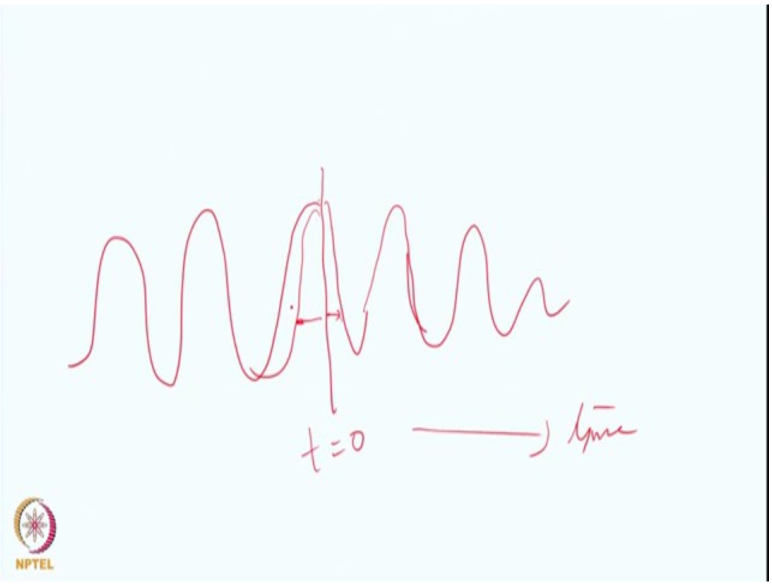

So if we have FID which is going like this, this is time $t=0$ and on this side it is going like this, this is time on the minus side, this is time t positive. If $f(-t)$, that means if I take a particular value of t here and a similar value of t if is symmetrical written here like this and if this values are same then it will mean f of t is equal to $f(-t)$that is a evenness. So if I have a cosine function this is what I get this is a cosine function is symmetrical with respect to t is equal to 0, therefore, if we have $f(t)=f(-t)$then your frequency domain spectrum.

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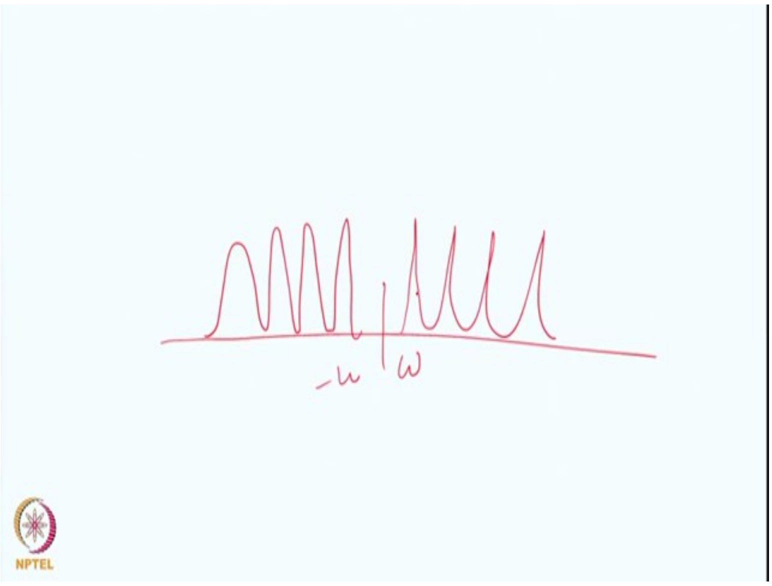

Draw the frequency domain spectrum this is $\omega=0$,you have the positive frequency here and you have the other frequencies here, if this is ω this is $-\omega$ and these two are equal. This is what we said if $f(\omega)=f(-\omega)$ the intensity of the signal is the same and it has the same sign. So that is what we get from the first theorem.

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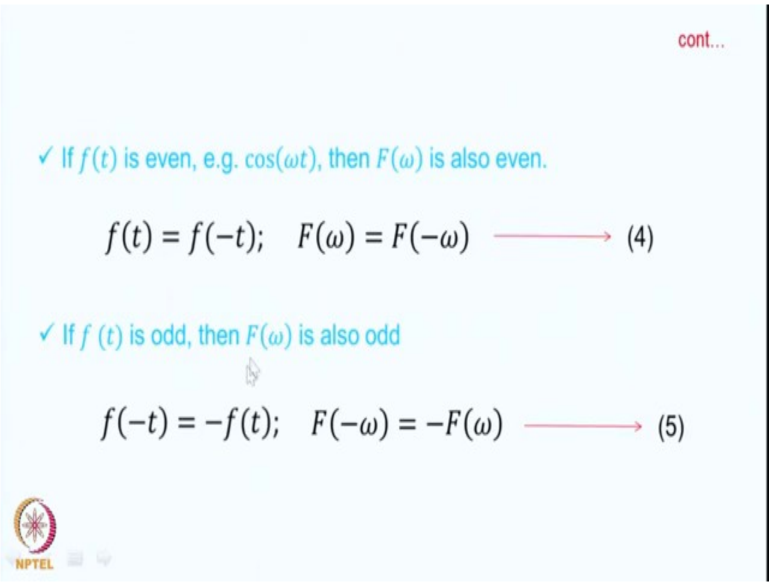

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$$f(t)=f(-t);\quad F(\omega)=F(-\omega) \longrightarrow (4)$$

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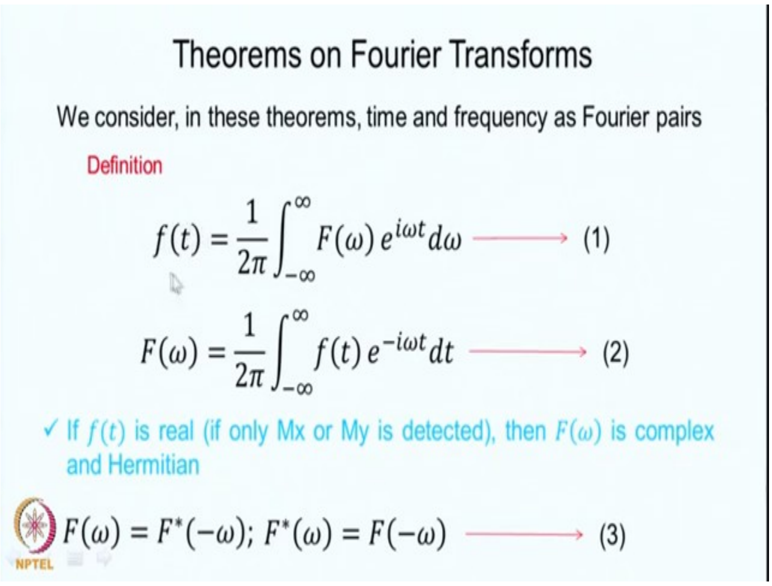
$$f(-t)=-f(t);\quad F(-\omega)=-F(\omega) \longrightarrow (5)$$



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✓ If $f(t)$ is real (if only Mx or My is detected), then $F(\omega)$ is complex and Hermitian

$$F(\omega)=F^{*}(-\omega);\ F^{*}(\omega)=F(-\omega) \longrightarrow (3)$$

Similarly, if $f(t)$ is odd that is when we consider a sine functions for example if

$f(t)=sin\omega t$, then $f(-t)=f(t)$, suppose this is $sin\omega t$, $sin\omega t$ if I changed *t* to *-t* then it becomes the $-sin\omega t$ and that is *f(-t),* in that case your frequency domain spectrum $f(-\omega)=f(\omega)$

So what was positive of both sides earlier than on one side it will be positive and the other side it will be negative. So this half of the spectrum if it is positive like this and the other side the spectrum will be negative like this that is minus f of mega ok, so that is what you will get if f of t is odd, how do we get such kind of situation? This depends upon what we actually collect, if we collect only one of this components “M_x” or “M_y” depending upon what you collect this can be collected as a cosine function or a sine function and depending on that you will have this sort of behavior ok.

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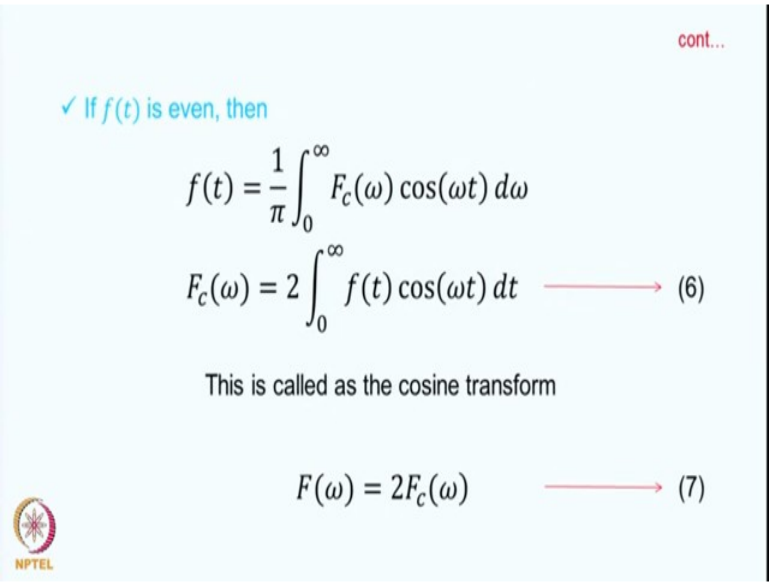

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✓ If $f(t)$ is even, then

$$f(t) = \frac{1}{\pi}\int_0^\infty F_c(\omega)\cos(\omega t)\,d\omega$$

$$F_c(\omega) = 2\int_0^\infty f(t)\cos(\omega t)\,dt \longrightarrow (6)$$

This is called as the cosine transform

$$F(\omega) = 2F_c(\omega) \longrightarrow (7)$$

Now, there are other properties which will come as a result of the definition of Fourier transform itself.

$$f(t) = \frac{1}{\pi}\int_0^\infty F_c(\omega)\cos(\omega t)\,d\omega$$

Now this function, $F_c(\omega)$ is called as a cosine transform.

$$F_c(\omega) = 2\int_0^\infty f(t)\cos(\omega t)\,dt$$

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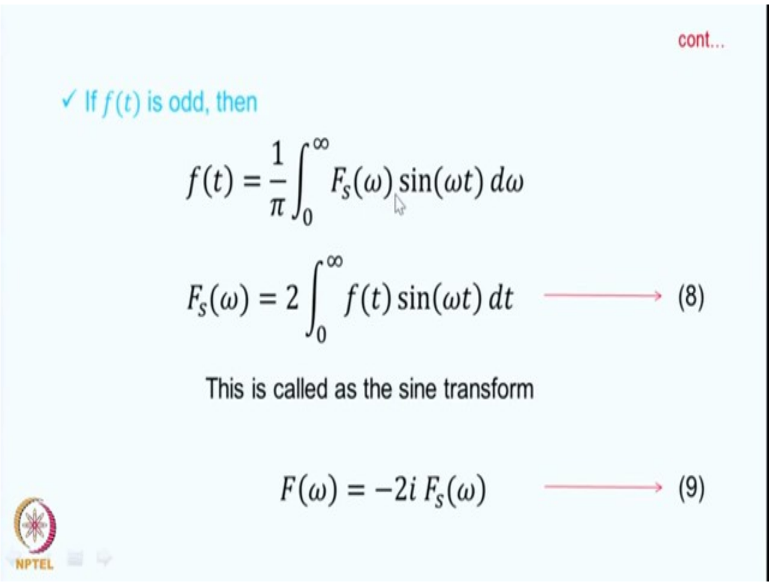

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✓ If $f(t)$ is odd, then

$$f(t) = \frac{1}{\pi}\int_0^\infty F_s(\omega)\sin(\omega t)\,d\omega$$

$$F_s(\omega) = 2\int_0^\infty f(t)\sin(\omega t)\,dt \longrightarrow (8)$$

This is called as the sine transform

$$F(\omega) = -2i\,F_s(\omega) \longrightarrow (9)$$

Likewise if $f(t)$ is odd, $f(t)$ is odd that means $f(t)$, $f(-t) = f(t)$ and that happens when we have $f(t)$ as a sine function. For example here as I can say that here is a sine function, in this situation f of t can be written as

$$f(t) = \frac{1}{\pi}\int_0^\infty F_s(\omega)\sin(\omega t)\,d\omega$$

And

$$F_s(\omega) = 2\int_0^\infty f(t)\sin(\omega t)\,dt$$

Now this function is called as the sine transform and here one can also prove then following the main definition

$$F(\omega) = -2i\,F_s(\omega)$$

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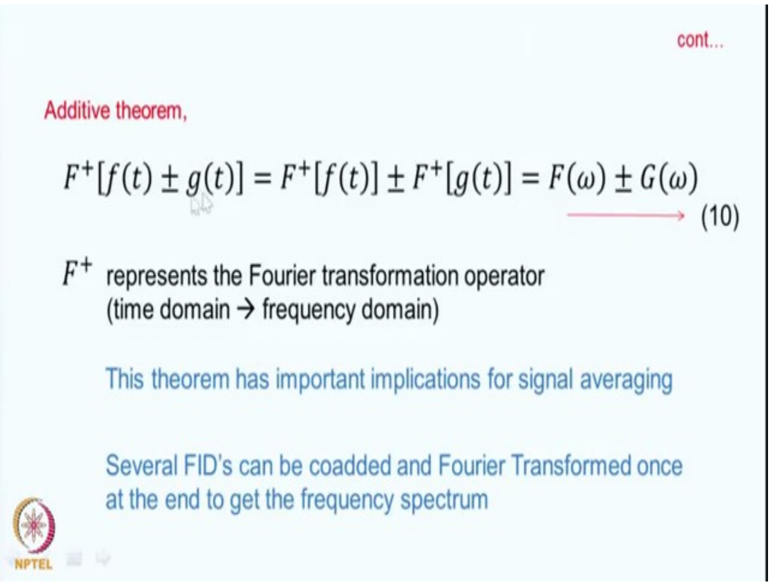

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Additive theorem,

$$F^{+}[f(t) \pm g(t)] = F^{+}[f(t)] \pm F^{+}[g(t)] = F(\omega) \pm G(\omega) \xrightarrow{\quad} (10)$$

F^{+} represents the Fourier transformation operator
(time domain → frequency domain)

This theorem has important implications for signal averaging

Several FID's can be coadded and Fourier Transformed once at the end to get the frequency spectrum

The next theorem we will like to consider which will follow from again from the definitions so this one can work it out explicitly. Suppose I have two functions,

$F^{+¿}[f(t)\pm g(t)]=F^{+¿[f(t)]\pm F^{+¿[g(t)]=F(\omega)\pm G(\omega)¿}¿}¿$

$f(t)$and $g(t)$ they may represent for example two different FIDs on the same sample once you collected and then we collected once more you essentially like signal averaging, so you collect two times the function f of t and then you can add or subtract g of t that is the both or two FID's added here, then we take the Fourier transform of these total time domain function what you get here. This is equivalent to taking the Fourier transform of this function, plus or minus the Fourier transform of the second function.

So therefore, it the sum or the difference of the Fourier transforms of the individual function. Now $F(\omega)$ is the Fourier transform of $f(t)$ and $G(\omega)$ is the Fourier transform of $g(t)$. Therefore, if I add is these two time domain function the Fourier transform of the whole thing is equal to the sum or the difference of the Fourier transforms of individual functions, and here noticed that the $F^{+¿¿}$ represents the Fourier transform operator, that is going from time domain to frequency domain, these operates in the time domain function and the result what we get is frequency domain function.

This theorem has important implication for signal averaging, see the question is when we want to add the signals in the spectra do you add them in the frequency domain or in the time domain? If we were do it in the frequency domain every time we will have to do the Fourier transform store it and then we add it.

Now which is a more time consuming process? The Fourier transformation takes the several seconds, whereas the data equitation takes few hundred milliseconds, if we have to do Fourier transform every time with the FID and then we add the frequency domain it will we very very time consuming, of course not as time consuming as slow passage but nonetheless it will take much more time than if we add simply in the time domain itself you add the various FID’s one after the other add them hundred times each one them is few hundred milliseconds you collect all there FID’s together and add them and then you do Fourier transformation once at the end.

So that means it will be a great saving in the time and therefore, the signal in to noise per unit time will be further enhanced as a consequence of this. Therefore, this is an important theorem from the point of view of signal averaging.

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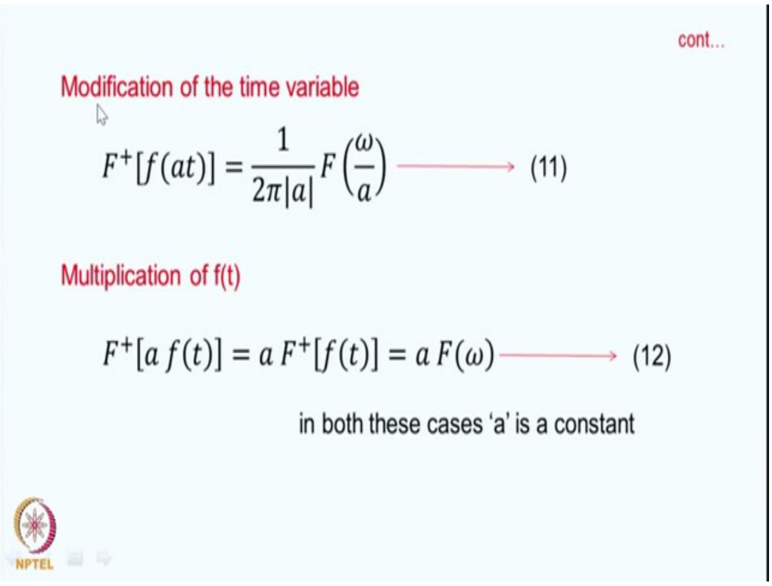

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Modification of the time variable

$$F^{+}[f(at)] = \frac{1}{2\pi|a|} F\left(\frac{\omega}{a}\right) \longrightarrow (11)$$

Multiplication of f(t)

$$F^{+}[a\,f(t)] = a\,F^{+}[f(t)] = a\,F(\omega) \longrightarrow (12)$$

in both these cases ‘a’ is a constant

Now, if you modify the time variable for example, you have a function f of t earlier what we considered, we are taking a Fourier transformation.

$F^{+¿[f(at)]=\frac{1}{2\pi|a|}F\left(\frac{\omega}{a}\right)¿}$

You can easily verify using this equation the properties which we described with respect to the evenness of the time domain function or the evenness of the frequency domain function. Suppose I put $a=-1$ here, then *f(-t)* what will happen here? *f(-t)* and this is the modulus here therefore, it does not matter and here it is $\frac{\omega}{a}$, $a=-1$ this will become equal to *-1*.

Therefore,

$F^{+¿[af(t)]=aF^{+¿[f(t)]=aF(\omega)¿}¿}$

So this is like when you are doing an experiment you enhance the gain, this is so called gain so if you multiply the entire function by a constant, then your entire frequency domain spectrum will be multiply by the same constant "a".

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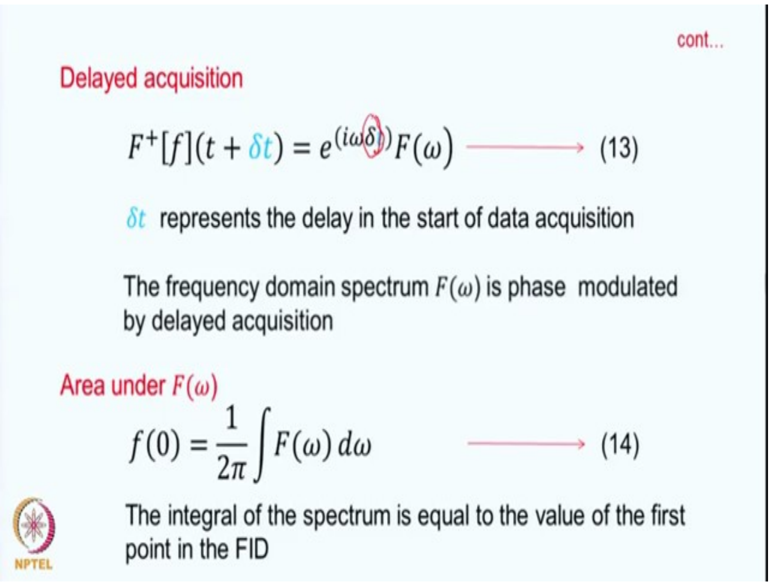

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Delayed acquisition

$$F^{+}[f](t+\delta t)=e^{(i\omega\delta t)}F(\omega) \longrightarrow (13)$$

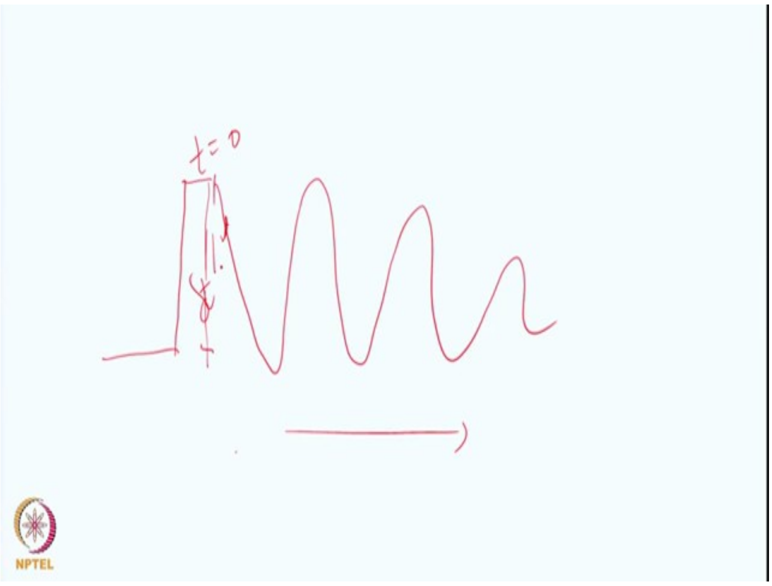
δt represents the delay in the start of data acquisition

The frequency domain spectrum $F(\omega)$ is phase modulated by delayed acquisition

Area under $F(\omega)$

$$f(0)=\frac{1}{2\pi}\int F(\omega)\,d\omega \longrightarrow (14)$$

The integral of the spectrum is equal to the value of the first point in the FID



Delayed acquisition, so here is the new property what we have and this notice here I would like to say something here this is one term δt, this is δt is one, unfortunately when we made this t has come in a different colour and δ has come in a different colour, but that is not what it is supposed to be δt this δt which is present here is the same one should be there. It is not the product of the δ in t, it is δt is one entity.

So δt represents the delay in the sort of data acquisition what that this mean? I have the FID which is going like this. So this was my time t is equal to 0, suppose I do not start the acquisition from time $t=0$, but I start from somewhere here and this period is δt. I give a delay, I give a delay in the data acquisition although I should have collected from here because when I apply the pulse if I apply the pulse immediately after the pulse I should start collecting the data, as soon as I remove the RF that is the time $t=0$ and then I should start collecting the data from there.

But however, if I wait for some time and insert the delay there that means I do not start the acquisition from here, but I started acquisition from there, so this time is δt what is the consequence of that?

$F^{+¿[f]|(t+\delta t)=e^{|i\omega\delta t|}F(\omega)¿}$

And noticed this depends up on the frequency here and depending upon what δt is at the different frequency we will have different phase factor, therefore, we have a frequency dependent introduction of the phase of the frequency spectrum, And this of course one has to get rid of it, these are the issues which come as a result of the Fourier transformation.

So therefore they are very for a Fourier transform NMR and this thing we will discuss at the later stage as to how to correct this for various purposes. Delta t represents the delay in the start of data acquisition as I explained to you. The frequency domain spectrum is phase modulated by delayed acquisition.

Now, from the definition of the Fourier transform we also will realize that *f (0)* that is if time $t=0$ what we get here?

$$f(0)=\frac{1}{2\pi}\int F(\omega)d\omega$$

Now, what this integral means? This integral means this is the total area under the curve, this is the total are under the spectrum the integral of the spectrum is therefore, equal to the value first point in the FID, the FID as you remember is going like this, the first point in the FID is your f of 0, and that value is equal to the total integral of the frequency domain spectrum, this is important application once again for various purposes.

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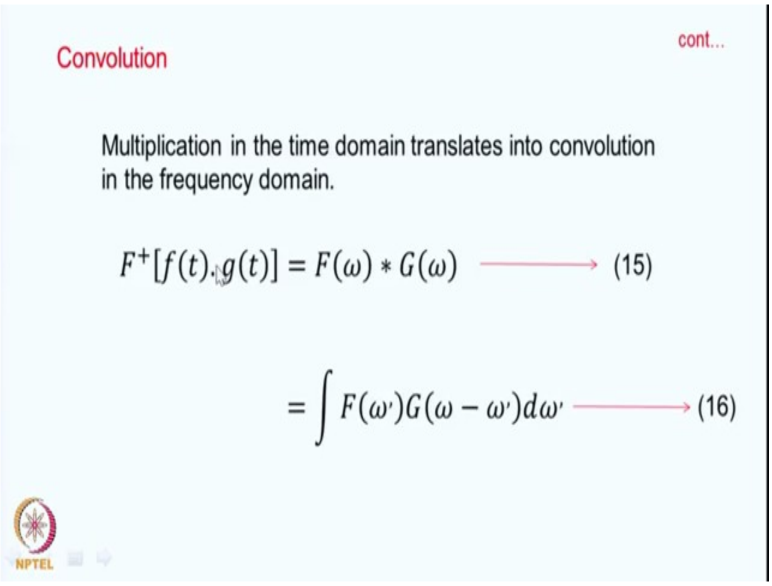

Convolution

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Multiplication in the time domain translates into convolution in the frequency domain.

$$F^{+}[f(t).g(t)] = F(\omega) * G(\omega) \longrightarrow (15)$$

$$= \int F(\omega')G(\omega - \omega')d\omega' \longrightarrow (16)$$

Now, multiplication in the time domain translates into the convolution into the frequency domain. These is another mathematically operation called convolution. Now we looked at what happens if we do addition of two FID's we therefore, then we said that it is a result will be sum of the two Fourier transforms.

In this, suppose we were to consider a multiplication here *f(t)* multiplied by *g(t)* there is another function this is like modifying in the FID in some manner, so in that case what happens this is this the two individuals Fourier transforms we calculate and then we take a convolution of these two of this functions. The convolution is an operation which is defined in this manner

$F^{+¿[f(t).g(t)]=F(\omega)*G(\omega)=\int F(\omega')G(\omega-\omega')d\omega'¿}$

So this is often used to simplify your spectra remove some of the artifacts but did also has an implication for actual data collection as we will see in the next theorem. And that is called as digitalization.

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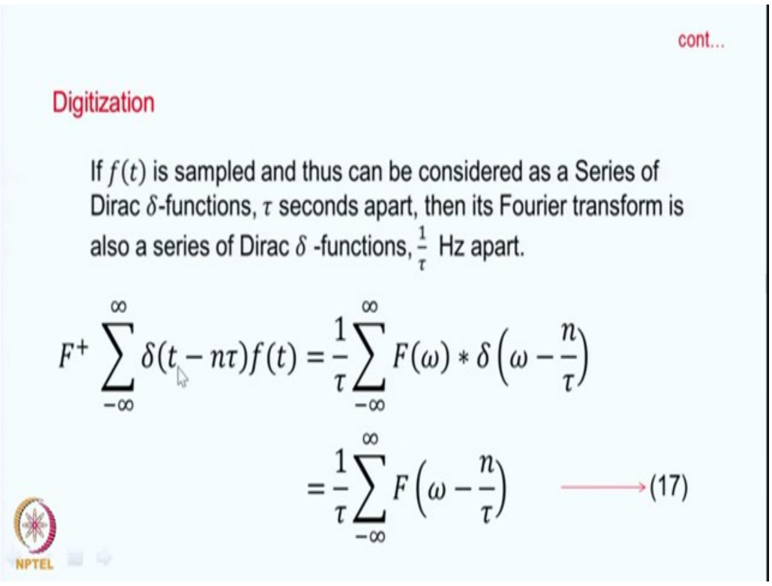

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Digitization

If $f(t)$ is sampled and thus can be considered as a Series of Dirac δ-functions, τ seconds apart, then its Fourier transform is also a series of Dirac δ -functions, $\frac{1}{\tau}$ Hz apart.

$$F^{+}\sum_{-\infty}^{\infty}\delta(t-n\tau)f(t)=\frac{1}{\tau}\sum_{-\infty}^{\infty}F(\omega)*\delta\left(\omega-\frac{n}{\tau}\right)$$

$$=\frac{1}{\tau}\sum_{-\infty}^{\infty}F\left(\omega-\frac{n}{\tau}\right) \longrightarrow (17)$$

Digitalization means that your FID is an analog signal it is a continue signal which is coming as in this manner, but we collects the signal in a continuous manner. Suppose, we were collect the data as a series of Dirac δ function, the words we collect the points at certain time intervals, then its Fourier transform is also a series of Dirac δ functions, $\frac{1}{\tau}$ hertz apart, mathematically it is represent in this manner

$$F\sum_{-\infty}^{\infty}\delta(t-n\tau)f(t)=\frac{1}{\tau}\sum_{-\infty}^{\infty}F(\omega)*\delta\left(\omega-\frac{n}{\tau}\right)$$

So each term here represents one data point so as n increases you get a different data points a summation of all of this essentially is a arranging all of this points at different time intervals and that is your FID.

So if I take the Fourier transform of that then from the previous theorem I get the convolution of this Fourier transform of this function and the Fourier transform of this function so that I get a convolution of these two frequency domain spectra and eventually that is represented in this manner,

¿ $\frac{1}{\tau}\sum_{-\infty}^{\infty}F\left(\omega-\frac{n}{\tau}\right)$

So this is a series of spectra what it implies is, there is series of spectra which are separated by $\frac{1}{\tau}$ and this has important implications later as we see for the folding of signal and so on.

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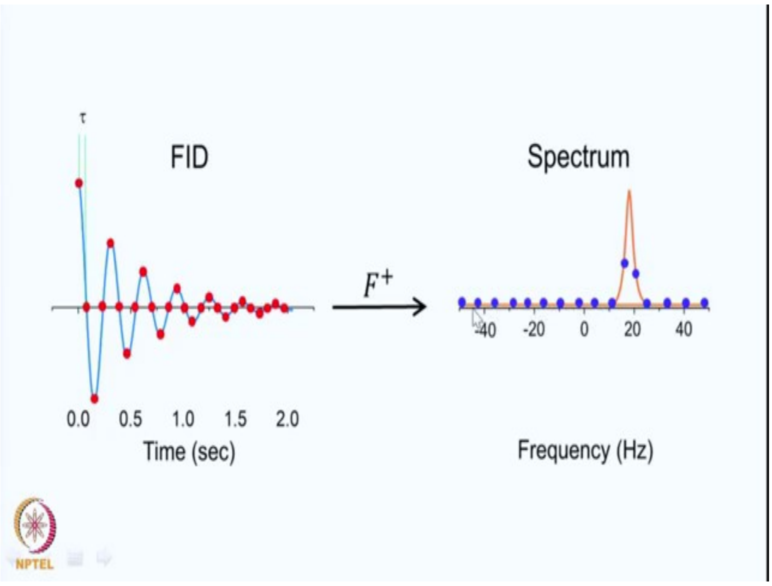

So this is schematically indicated here for your easy understanding, this FID was like this we are not collecting the FID in this manner, we collect the FID as a series of points and the time between two consecutive points is tau this is called as a dwell time and this is also represented as sampling. So, how you sample your FID? You collect the data here, a point here and a point here and a point here and a point there.

So this is called as sampling, so you collects the data points systematically over the entire FID and then what you get after the Fourier transform such a discrete data set you will get a spectrum which also is a discrete set of points, so you do not have an analog signal which is this curve here, but you get points like this which are equally spaced and then you connect those and extrapolate in between to generate your frequency domain spectrum.

Therefore, how well you represent your data, your spectrum here depends up on how well this points are separated, how close they are, closer they are the better is the representation of your spectrum therefore, all this is things are important with regard to the spectral resolution in the data sets.

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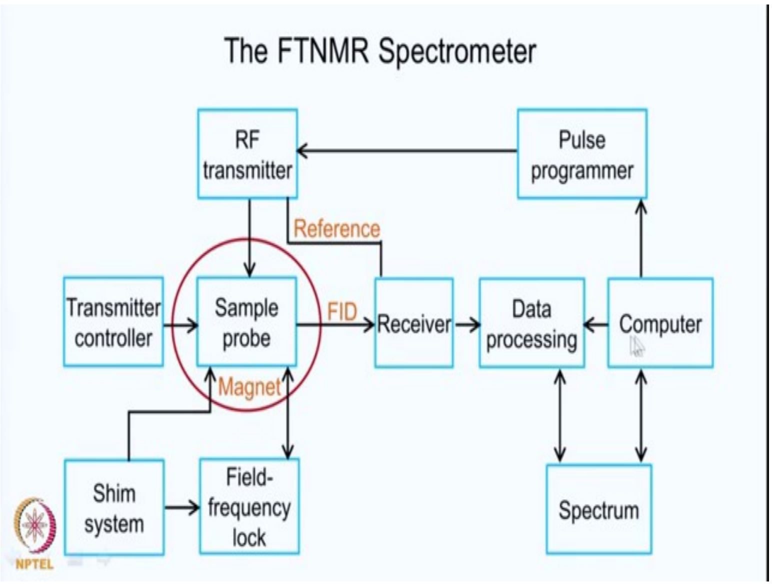

The FTNMR Spectrometer

So therefore, with all of this we now look at the FTNMR spectrometer what are the integral important elements of this. Of Couse the magnet and all of those things remains as they were before, but we have certain essential improvements or essential elements which are present here, because now the whole thing has to be very highly and precisely controlled. So therefore, the new elements come in the picture here we have the transmitter controller as before the shim system, the field frequency lock, the sample probe this lies in the magnet and today we can magnets of the different a types.

We have super conducting magnets which can produce very high magnetic fields which have very high stabilities and then we have the RF transmitter which produces the pulse and we have this RF frequencies also applied to the receiver here which means we actually detect the signal in the rotating frame, this basic transmitter frequency omega naught is attracted here from the signal what we are collecting from the sample and therefore, it amounts to saying that we are collecting the signal in the rotating frame.

And then we do data processing, data processing means you collect the FID here therefore, you will have to do the Fourier transformation and that becomes the data processing. All these requires the computer, why do we need the computer? Because you need your precise control, you will have the pulse the pulse programmer here which generates the pulse RF pulse and sends it here.

The pulse programmer means you apply a pulse which is of the order of microseconds 10 microseconds, 10.2 microseconds, 1.2 microseconds, so that precision is required timing control is required and therefore the time integral element of spectrometer will be the computer, the computer can manage all of this and then finally after data processing you have the spectrum.

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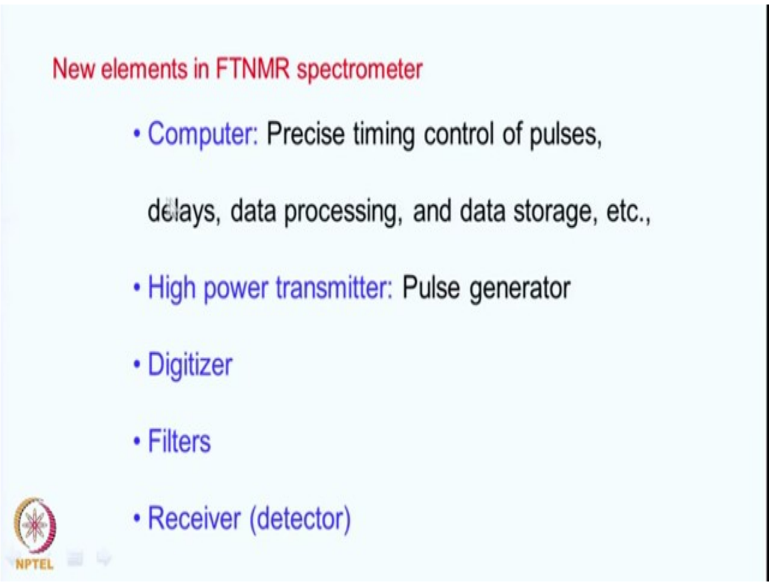
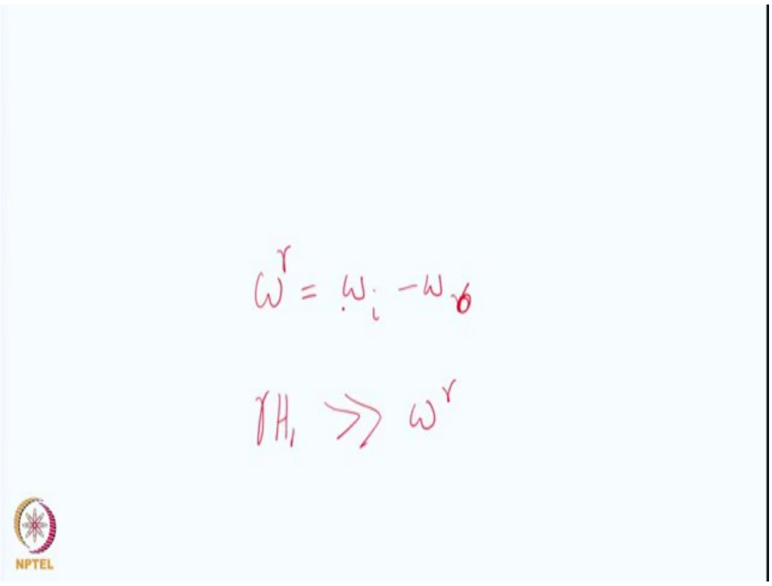


New elements in FTNMR spectrometer

- Computer: Precise timing control of pulses, delays, data processing, and data storage, etc.,
- High power transmitter: Pulse generator
- Digitizer
- Filters
- Receiver (detector)



$$\omega^r = \omega_i - \omega_0$$

$$\gamma H_1 \gg \omega^r$$

So if have to summarize this in words, you have the computer control is essential, precise timing control of pulses, delays because you need to know how much delay you have given because we see the delay equalization leads through phase modulation of the spectrum and therefore, you need to know how much delay you have put and we should be precise and we need to know exactly how much is that? Data processing, and data storage, etc.

Now, if I want to collect the data apply *RF* pulse so that I excite all the spins at the same time. You remember we have to apply the high power transmitter, why do we need high power? And this is because our γH_0which is our effective field has to be much larger than all the frequencies in the rotating frame. So let me put that back to you here so recall that once more.

So we have a rotating frame frequency $\omega^r = \omega_i - \omega_0$,and this can be of the order of several kilohertz $\omega_i - \omega_0$, this is the *RF* frequency this is the frequency of your precision and we said in the effective field γH_1 should be much larger than the ω^r. So if this is of the order of 5000 hertz that is if we collect a protons spectral range of 10 ppm for 100 megahertz it is 1000 hertz, for a 500 megahertz NMR spectrometer this is 5000 hertz.

Now, if I had to have the same effective fields for the entire set of spins we said that gamma H1 should be much larger than omega r. So if this were 5 kilohertz then I should have this one at least 20 kilohertz or 25 kilohertz that kind of a range I must have.

So therefore, high power transmitter is required and that, this is a pulse generator.

Then, we need a digitizer, digitizer means the signal that comes out from NMR sample is an analog signal, but we have to consider points because we now collecting data at the certain intervals as a systematically placed time intervals and therefore, we need a digitizer. The digitizer converts the analog signals in to the digital signal that means the signal will be a set of points as indicated earlier.

Then we need to have the filters, the filters are required to remove the unwanted frequencies that we will already mentioned that when we have the excitation in the sink pulse, we take the selective central RF excitation going like this and we had a small portion if you remember here we were to filter out that portion only and that requires filters and then we have the receivers, the receiver collects the signal, signal they are find this is also called as the detector, to this we also apply the main RF to go in the rotating frame so this also is a time domain signal which has to be collected at regular intervals of time and this will be the order of few hundred microseconds at the time points are collected at the intervals at several hundreds of microseconds depending upon the spectral width what we have. And how much you said be the how is the relation with respect to spectral width that will consider in the next classes.

So these are the essential elements which have become important as a result of the Fourier transform process of the excitations and data collection. We will stop here, and will continue with the further aspects of FTNMR and what are the features which are very specific to Fourier transform NMR in the next class, thank you.