

Signal detection, Fouriertransformation, phase correction and quadrature detection

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Schmilka 2004



What is this seminar about ?

Signaldetection

What kind of signal do we detect in NMR

Fouriertransformation

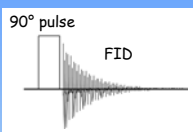
How is the time dependent signal transformed into a spectrum

Phase correction

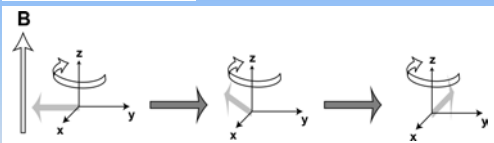
Why is a phase correction necessary

Quadratur detection

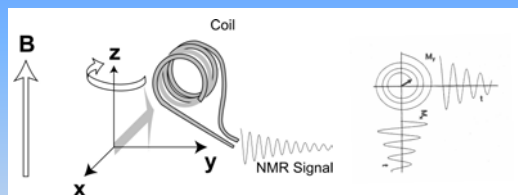
Why do we need quadrature detection



The simplest experiment in FT-NMR consists of one pulse and detection of an FID



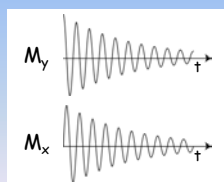
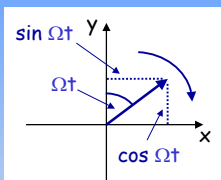
After the pulse magnetization starts to precess around the z-axis, i.e. the main magnetic field



This precession induces a current in the detection coil resulting in the signal that is recorded



An oscillating signal viewed from x and y axis results in a cosine and a sine dependency



$$M_y = \cos \Omega t \exp(-t/T_2)$$

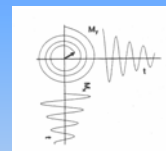
$$M_x = \sin \Omega t \exp(-t/T_2)$$



Both signals are detected to yield a complex NMR signal

$$M = M_y + i M_x$$

$$M = \exp(i\Omega t) \exp(-t/T_2)$$

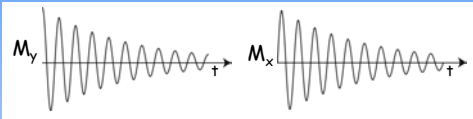


The above relation results from the famous Euler equations

$$\exp(i\alpha) = \cos \alpha + i \sin \alpha$$

$$\exp(-i\alpha) = \cos \alpha - i \sin \alpha$$



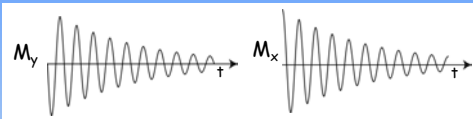
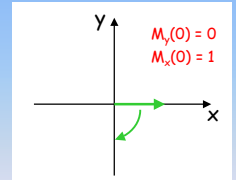
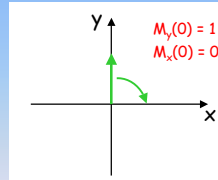


$$M_y = \cos \Omega_0 t \exp(-t/T_2) \quad M_x = \sin \Omega_0 t \exp(-t/T_2)$$

$$M = M_y + i M_x = [\cos \Omega_0 t + i \sin \Omega_0 t] \exp(-t/T_2)$$

$$M = \exp(i\Omega_0 t) \exp(-t/T_2)$$

We just saw the starting point of the precession at $M_y = 1$ und $M_x = 0$, but that is not a necessity



$$M_y = -\sin \Omega_0 t \exp(-t/T_2) \quad M_x = \cos \Omega_0 t \exp(-t/T_2)$$

$$M_y = -\sin \Omega_0 t \exp(-t/T_2) = \cos(\Omega_0 t + \pi/2) \exp(-t/T_2)$$

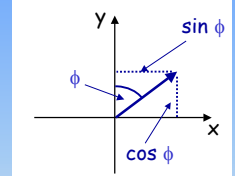
$$M_x = \cos \Omega_0 t \exp(-t/T_2) = \sin(\Omega_0 t + \pi/2) \exp(-t/T_2)$$

$$M = M_y + i M_x$$

$$M = \exp(i\Omega_0 t + \pi/2) \exp(-t/T_2)$$

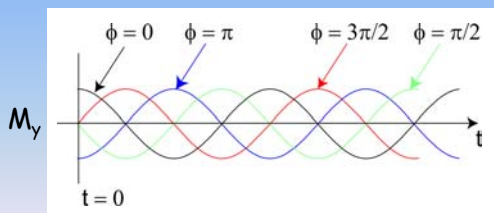
$$M = \exp(\pi/2) \exp(i\Omega_0 t) \exp(-t/T_2)$$

The starting position of the signal and the position of the detection axis are variable, the signal has a "phase"

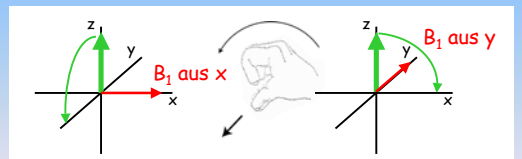


$$M = \exp(i\phi) \exp(i\Omega_0 t) \exp(-t/T_2)$$

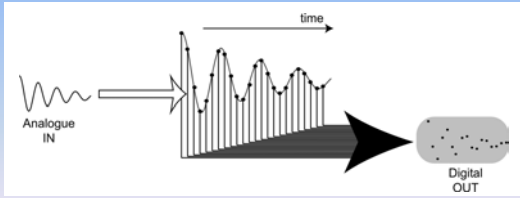
The phase tells us at which point of the wave the signal detection has begun



The phase can be influenced by the choice of the pulse phase but does also depend on the electronics (i.e. length of the cables)



To process the data on a computer using the DFT (discrete fourier transform) the signal needs to be digitized. The analog-to-digital-converter (ADC) does the job

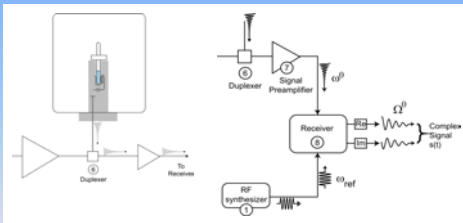


To make the digitization technically feasible the range of frequencies has to be as small as possible

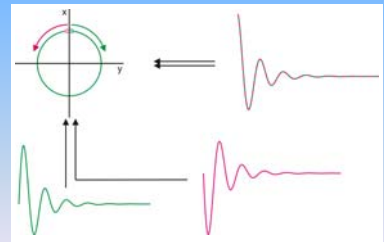
Therefore the original signal (sent as a pulse) is subtracted from the received signal to obtain only the modulation

In addition, the carrier is placed in the center of the spectrum allowing positive and negative frequencies (clockwise and counterclockwise rotation)

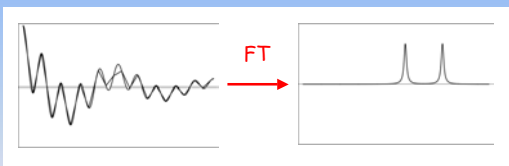
The detection unit



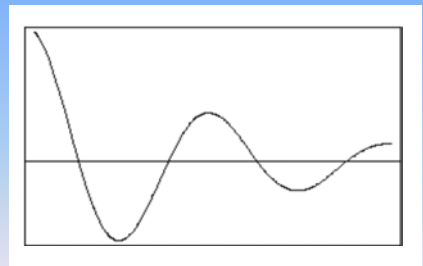
Putting the carrier in the center of the spectrum creates the need to distinguish positive and negative frequencies: quadrature detection



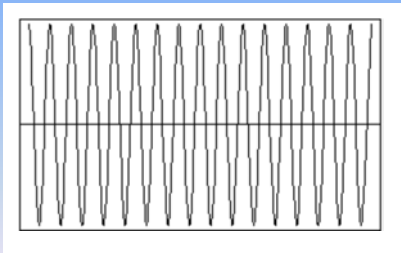
The FT transforms a mixture of time-dependent signals (oscillations) into a spectrum, which shows a frequency dependence



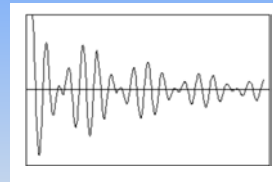
We want to know the frequency of the oscillation depicted below



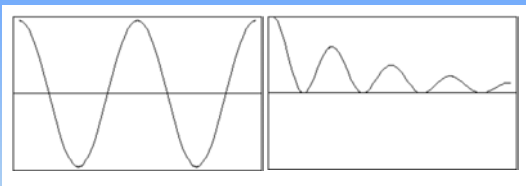
We start out with "guessing" a frequency



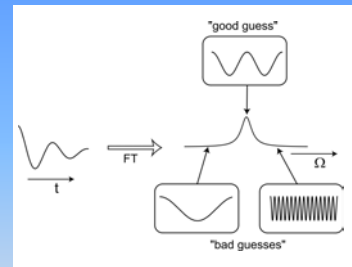
Then we multiply both and sum up all values of the resulting oscillation (i.e. we integrate)



If the frequencies do not match we get an equal amount of positive and negative values and the result is 0



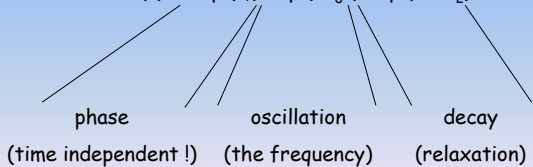
If the frequencies do match, most points will be positive and the result of the summation will be large



If we do this systematically for all possible frequencies, we obtain a „spectrum“ of all frequencies contained in the oscillation

Put in equations the easiest way to explain the FT is to use a complex function

$$s(t) = \exp(i\phi) \exp(i\Omega_0 t) \exp(-t/T_2)$$



We ignore the phase factor at first and do the multiplication and summation (integration)

$$S(\Omega) = \int_0^{\infty} s(t) \exp(-i\Omega t) dt$$

$$S(\Omega) = \int_0^{\infty} \exp(i\Omega_0 t) \exp(-t/T_2) \exp(-i\Omega t) dt$$

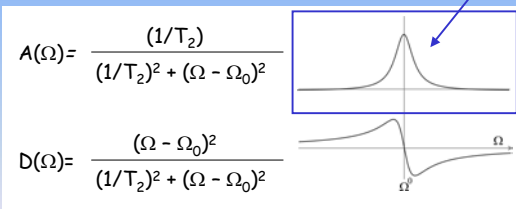
$$S(\Omega) = \frac{1}{(1/T_2) - i(\Omega - \Omega_0)} \quad \text{lorentian line}$$

A complex function consists of real and imaginary part

$$S(\Omega) = R(\Omega) + i I(\Omega)$$

In the simplest (and best) case the real part of an lorentian is absorbtive, the imaginary part dispersive
 $S(\Omega) = A(\Omega) + i D(\Omega)$

that's what we want



But we remember that the signal had a phase

$$S(\Omega) = [A(\Omega) + i D(\Omega)] \exp(i\phi)$$

$$S(\Omega) = R(\Omega) + i I(\Omega)$$

This makes real and imaginary part a mixture of the (desired) absorbtive and the (unwanted) dispersive part

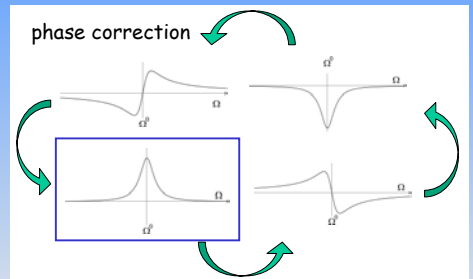
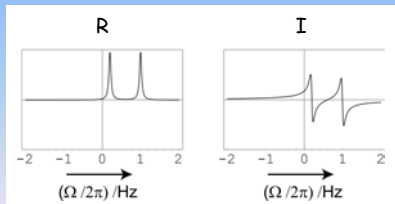
$$R(\Omega) = A(\Omega) \cos \phi - D(\Omega) \sin \phi$$

$$I(\Omega) = D(\Omega) \cos \phi + A(\Omega) \sin \phi$$

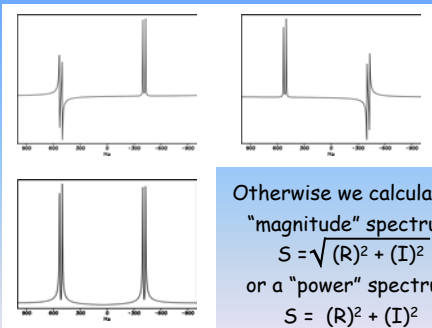
And that's what we correct by doing a phase correction

$$A(\Omega) = R(\Omega) \cos \phi + I(\Omega) \sin \phi$$

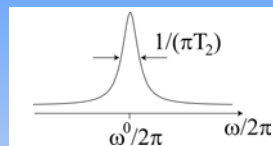
$$D(\Omega) = I(\Omega) \cos \phi - R(\Omega) \sin \phi$$



...which works as long as all signals have similar phase



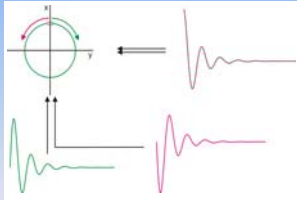
Otherwise we calculate a "magnitude" spectrum
 $S = \sqrt{(R)^2 + (I)^2}$
 or a "power" spectrum
 $S = (R)^2 + (I)^2$



$$s(t) = \exp(i\phi) \exp(i\omega^0 t) \exp(-t/T_2)$$

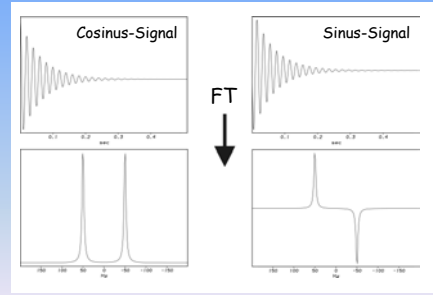
phase (time independent !)
 oscillation (frequency)
 decay (relaxation)

Recording a complex signal is essential not only for phase correction but also for quadrature detection

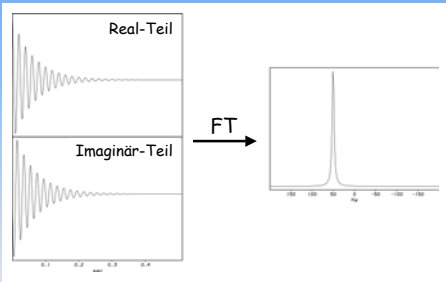


What if we would only record cosine and sine spectra
 $\cos\alpha = \exp(i\alpha) + \exp(-i\alpha)$
 $\sin\alpha = \exp(i\alpha) - \exp(-i\alpha)$

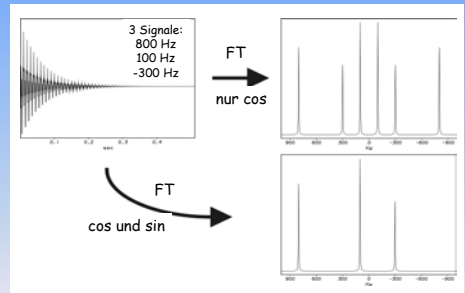
The result are two lines, the FT can then not distinguish between positive and negative frequencies



Which is why we have to combine both....



...to be able to put the carrier in the center of the spectrum



That's it