NMR course at the FMP:

Processing

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The program

The data structure

The digital filter

Window functions

Zerofilling

Linear prediction, Hilbert transform

NC_proc, xdim

The data structure

The data structure

Topspin requires a fixed data structure to be able to process data: DISK USER NAME EXPNO PROCNO

```
/x/data/guest/nmr/hsqc.090511/
        1/      fid
                acqu                                    (eda)
                acqus                                   (dpa)
                pdata/
                        1/              1r,1i
                                        proc            (edp)
                                        procs           (dpp)
```

and some other files

The data structure

```
/x/data/guest/nmr/hsqc.090504/
        2/      ser
                acqu
                acqus
                acqu2
                acqu2s
                        pdata/
                        1/              2rr, 2ri, 2ir, 2ii
                                        proc
                                        procs
                                        proc2
                                        proc2s
```

and some other files

The data structure

Higher dimensional data are build according to the same principle, the raw data are still stored in a serial manner thus the file is still a ser file

The processed data are 3rrr and 4rrrr, here it is advisable not to store the imaginary parts since they are quite big.

If necessary the imaginary part can be restored by a Hilbert transform

The data structure

Since 3D techniques are in principle constructed from 2D techniques it is possible to reduce a 3D to two 2Ds by keeping one of the indirect dimension fixed. Then „planes" are recorded, which is good test whether a 3D is going to work.

When processing a 3D it is also possible to first process the 2Ds individually as long as the acquisition dimension is one of the 2. This can be helpfull to adjust phases

The data structure

The data are stored as 32 bit (4 byte) integer data

That means an FID recorded with 4096 points will have a size of 16384 byte (16 kb)

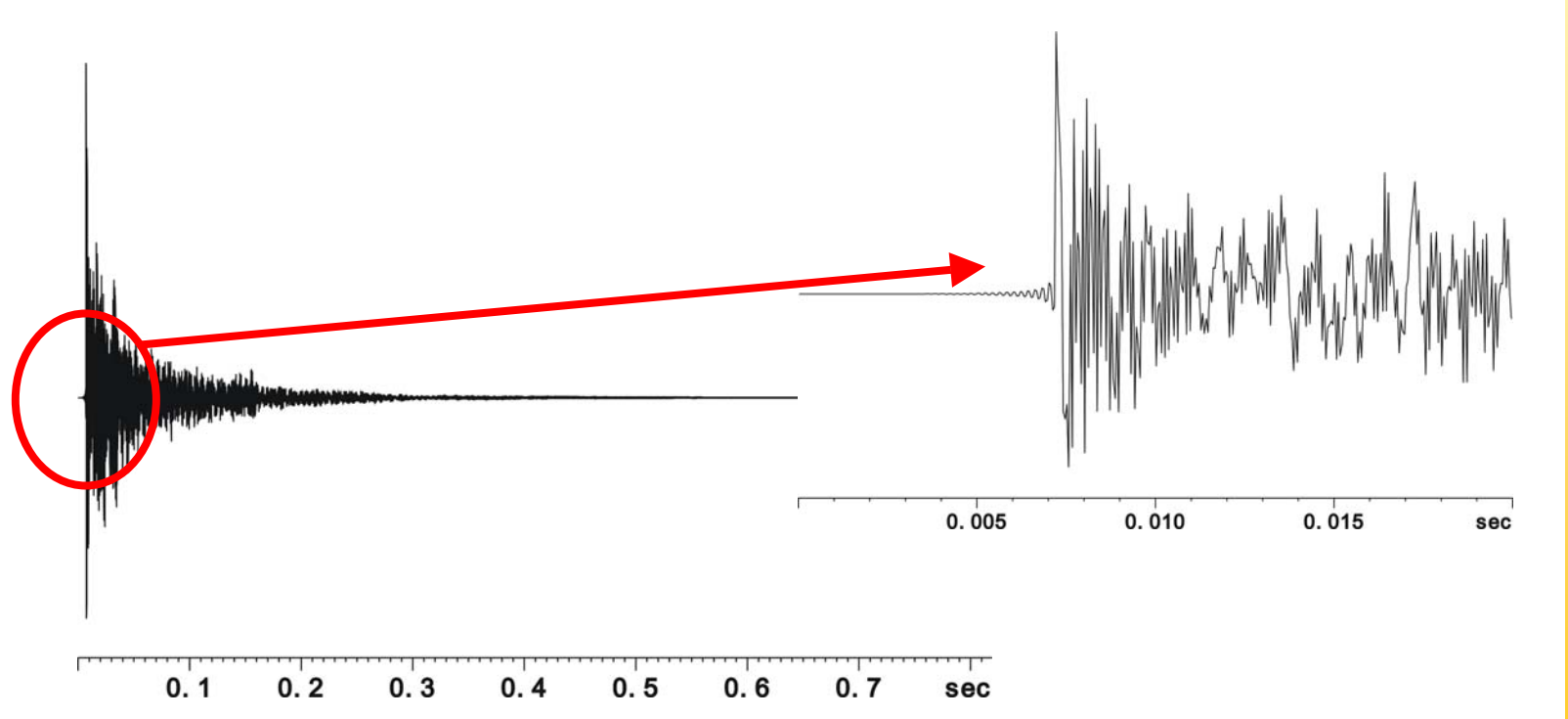
A SER file recorded with 512 FIDs of 4096 points each will have a size of 8388608 byte (8 Mb)

The size of the SER file is not changed if the experiment is stopped prematurely

The digital filter

The digital filter

Since over a decade bruker uses a digital filter to record the data. To remove it use „convdta“



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The digital filter

Most alternative programs are capable of reading Bruker data and handling the digital filter.

More modern spectrometer may produce differently filtered data, sometimes even topspin 1.3 can not read the data.

Certain operations may require conversion to analog

Zerofilling

and the mystery of TD and SI

Zero filling

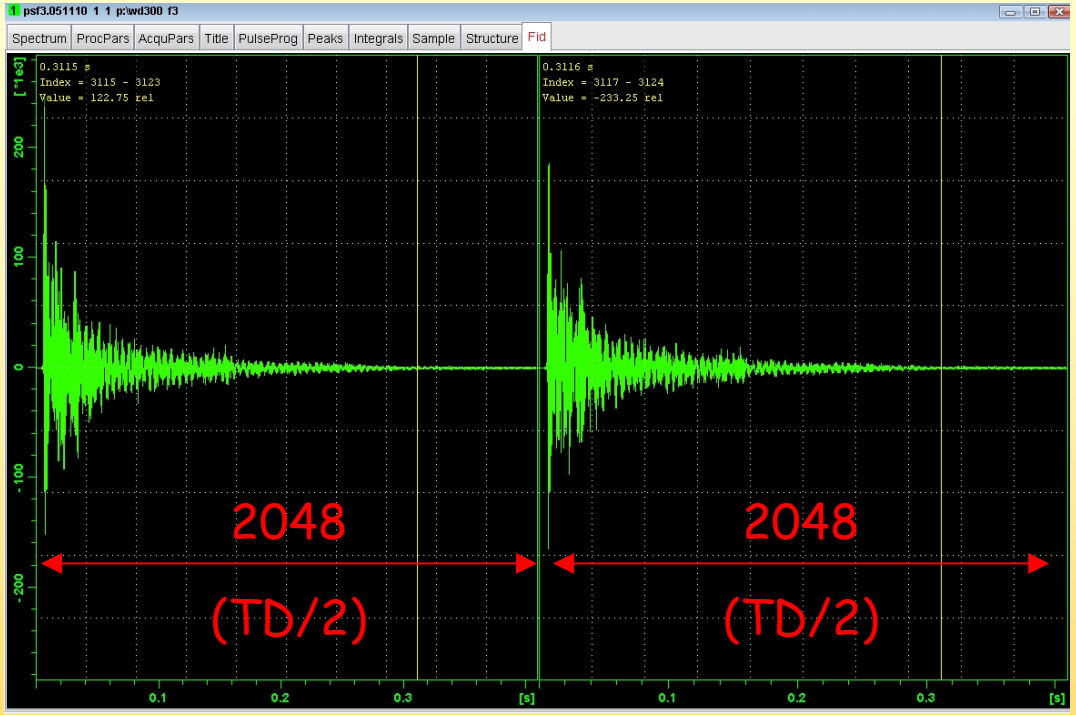
Zerofilling is a procedure that simply adds zeros to the end of the recorded data which are then used in the DFT algorithm as if they were normal data.

This may be necessary for the DFT algorithm that only work with 2^n data points

It may enhance the information content (zerofilling by a factor of 2)

It may improve the *digital* resolution to give improved accuracy when determining frequencies

Zero filling



2048 complex data points are 2048 data points in the real part and 2048 in the imaginary part

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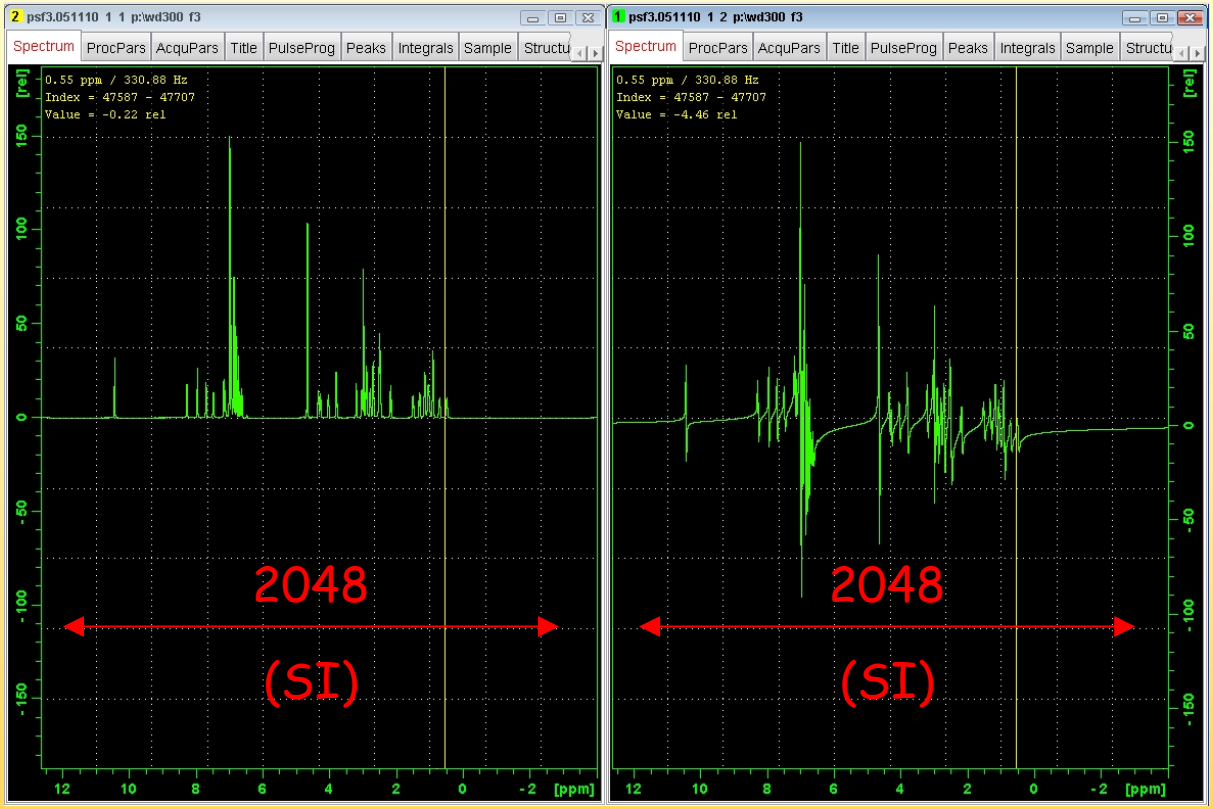
Zero filling



After an DFT we have 2048 data points in the real part and 2048 in the imaginary part

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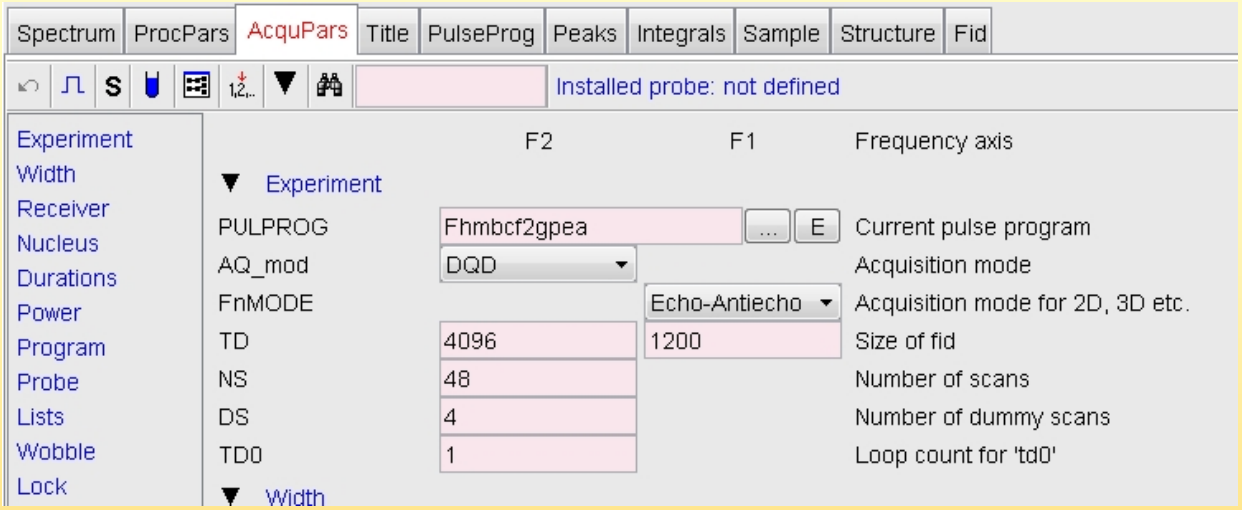
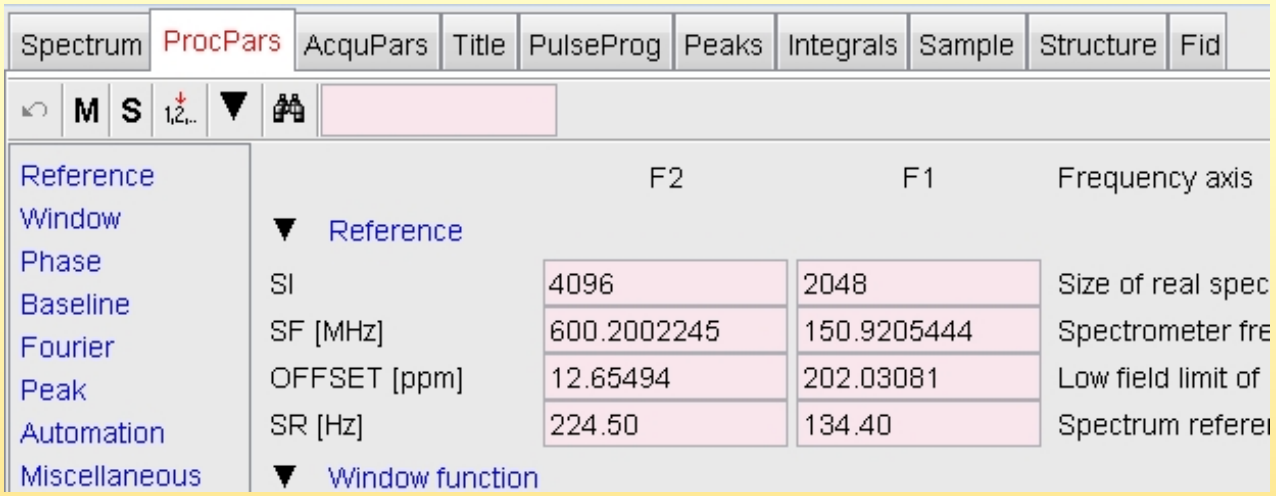
Zero filling



TD gives actual data points, 4096 thus corresponds to 2048 complex data points, 1200 FIDs are 600 complex points in the indirect dimension

Zero filling



SI does give real points. The DFT of an FID with TD=4096 results in a spectrum 2048 real and 2048 imaginary points. If we set SI to 4096 that means we have already zerofilled once, even though the numbers are identical

Zero filling

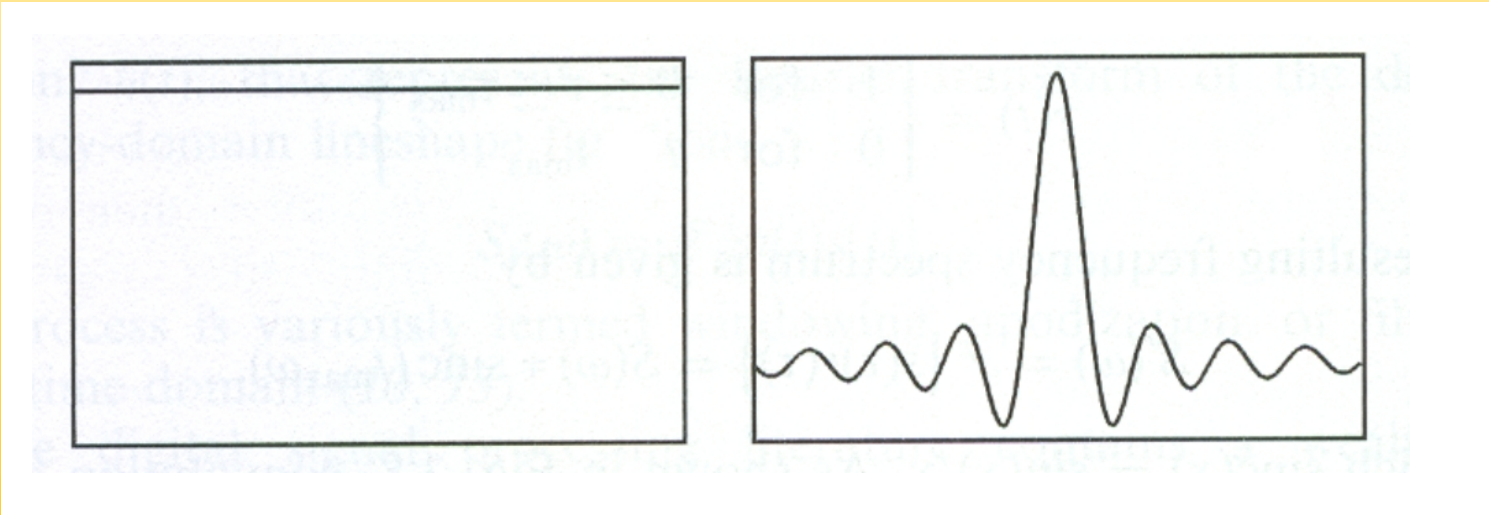
How many points should be recorded depends on the relaxation behaviour of the molecule. It may be better to cut the acquisition short and do zerofilling rather then recording only noise and entering it into the spectrum by a DFT. Zeros do contain less noise !

The number of FIDs should be adjusted to the achievable resolution, not to the desired one

Window functions

Window functions

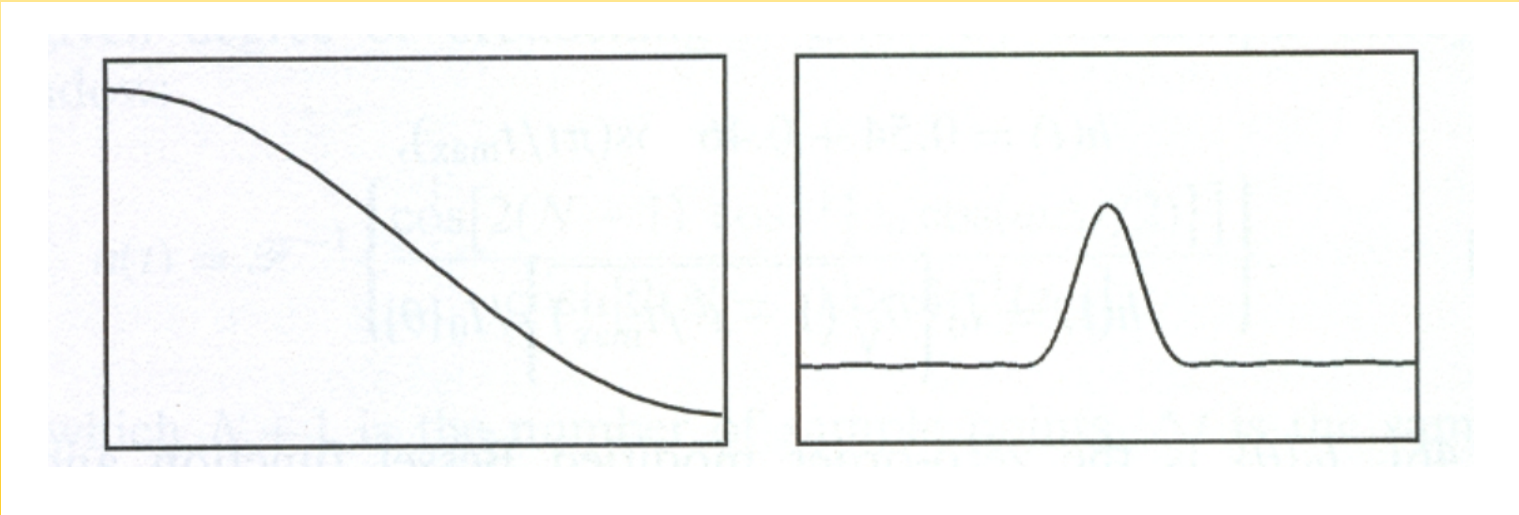
The application of window functions (also called "apodization") prior to the DFT helps to avoid artefacts resulting from shortcommings of the DFT and can help to improved the data



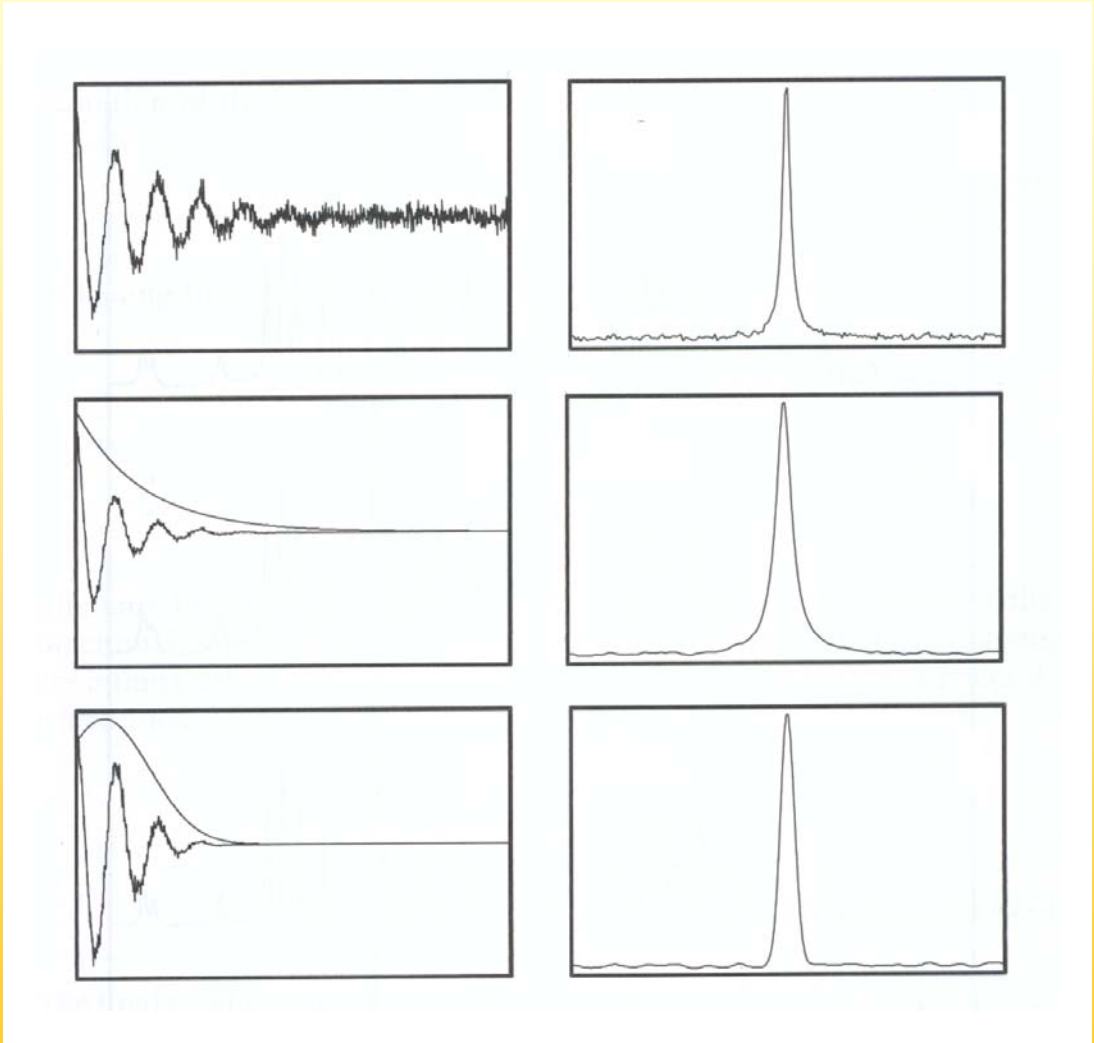
Window functions

A "standard window" function is the squared cosine, i.e. the FID is multiplied with a $(\cos(n*\Delta t))^2$

This does not change the intesity, it does also not improve the data, but removes artefacts from the DFT



Window functions



Two other popular functions are the exponential multiplication and the lorentz-to-gauss transformation

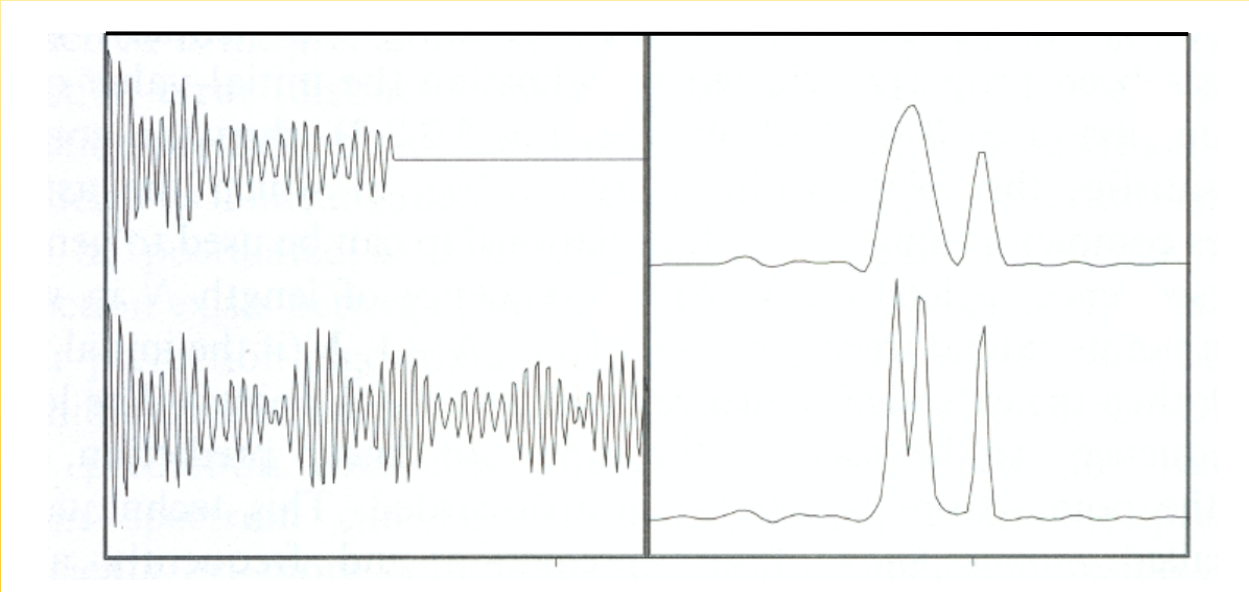
Linear prediction

Hilbert transform

NC_proc, xdim

Linear prediction

Using a mathematical procedure called "linear prediction", that is based on modelling the data using a system of linear equations, it is possible to extend the NMR data without using spectrometer time



Hilbert transform

Because of a mathematical relation between the real and the imaginary part of the NMR spectrum it is possible to reconstruct the imaginary part from the real one: the Hilbert transform.

This can be quite helpful if the imaginary part has been discarded after the DFT to save disc space.

The Hilbert tranform can then restore the imaginary part, that can be used for phasing and subsequently discarded again

NC_proc, xdim

NC_proc: Bruker uses integer as the data type. This forces them to scale the data at the end of the fourier transform. This is unnoticable when working within topspin, but if quantification has to be done outside topspin it my become relevant.

xdim: Bruker uses submatrices in their data structure, which can be relavant if converting processed data for other software. Normally, however, conversion programs can handle submatrices.

That's *not* it, we will now do some processing

www.fmp-berlin.de/schmieder/teaching/selenko_seminars.htm