

Overcoming line broadening in real-time pure shift NMR spectroscopy

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Plan

- Pure shift NMR: what for and how
- Line broadening in real-time pure shift NMR
- CS reconstruction as a remedy
- Details of CS: the idea and its realization
- Applications

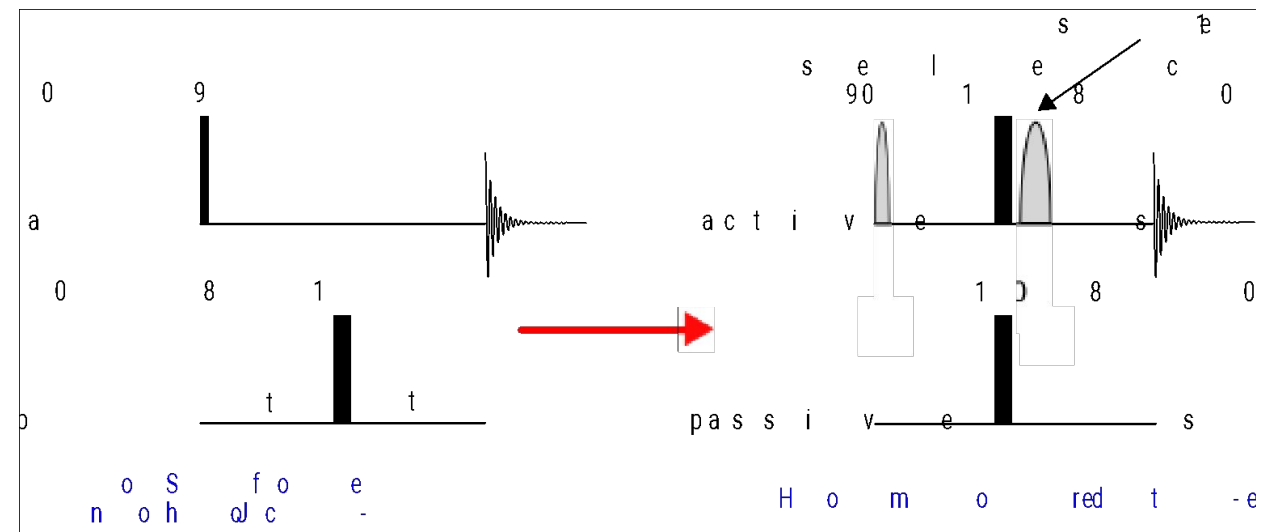
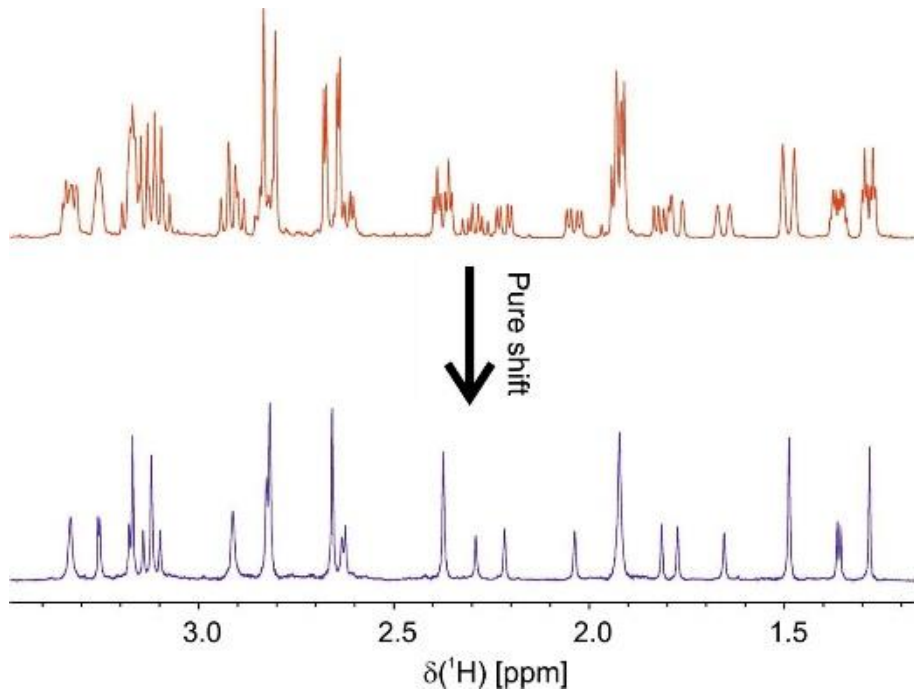
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Pure shift NMR as a tool for homodecoupling

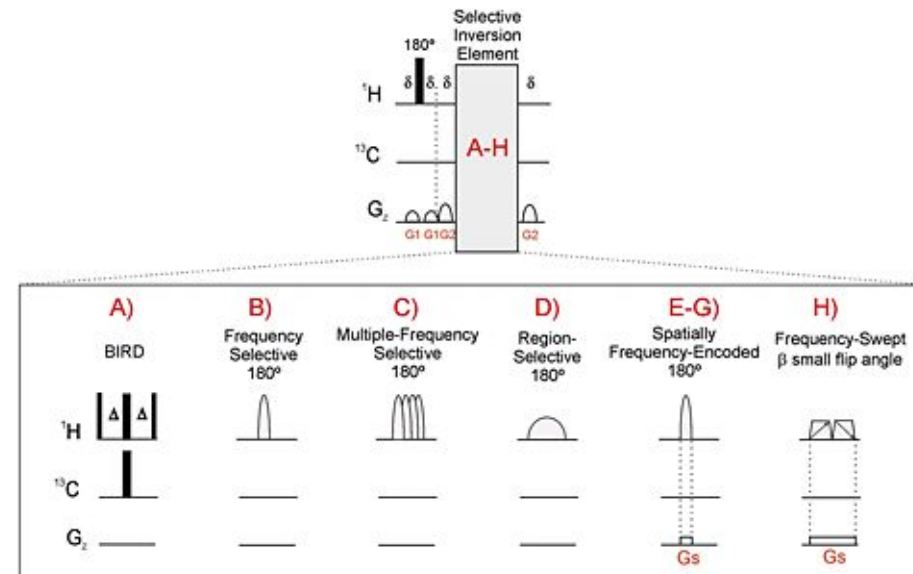
„For the practical spectroscopist it would be ideal if he could remove all spin-spin couplings at the same time”

Richard R. Ernst, 1963



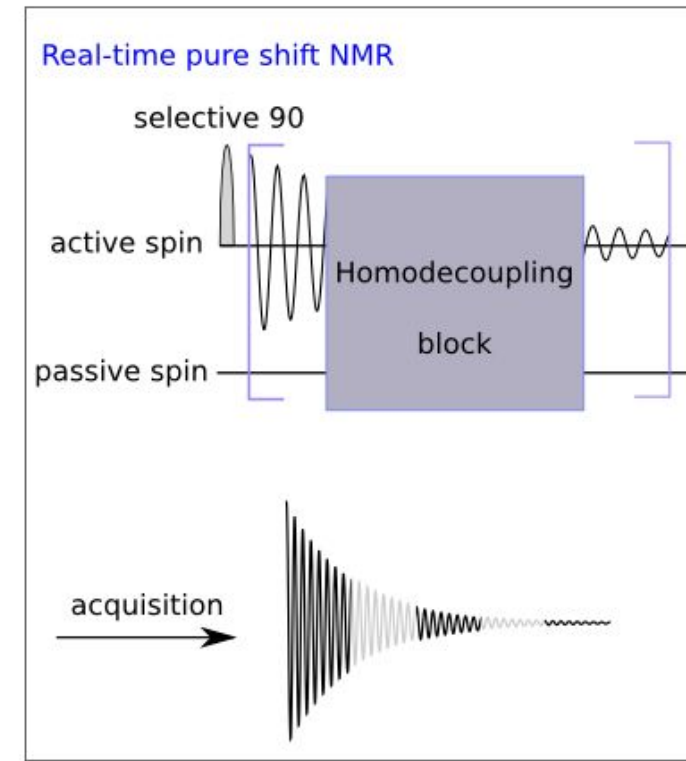
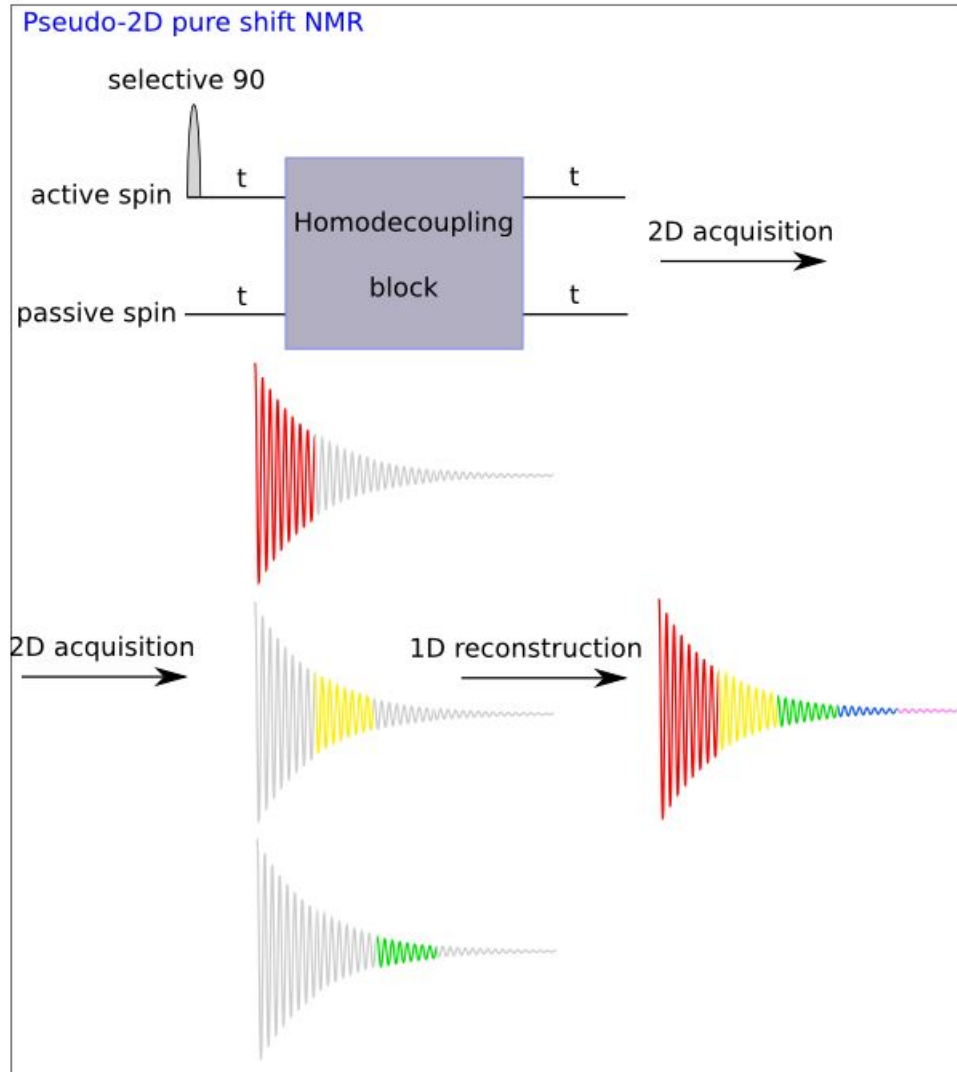
Selective pulses

- Spatially selective
or
- Frequency-selective
or
- BIRD-based pulse sequences
- ...



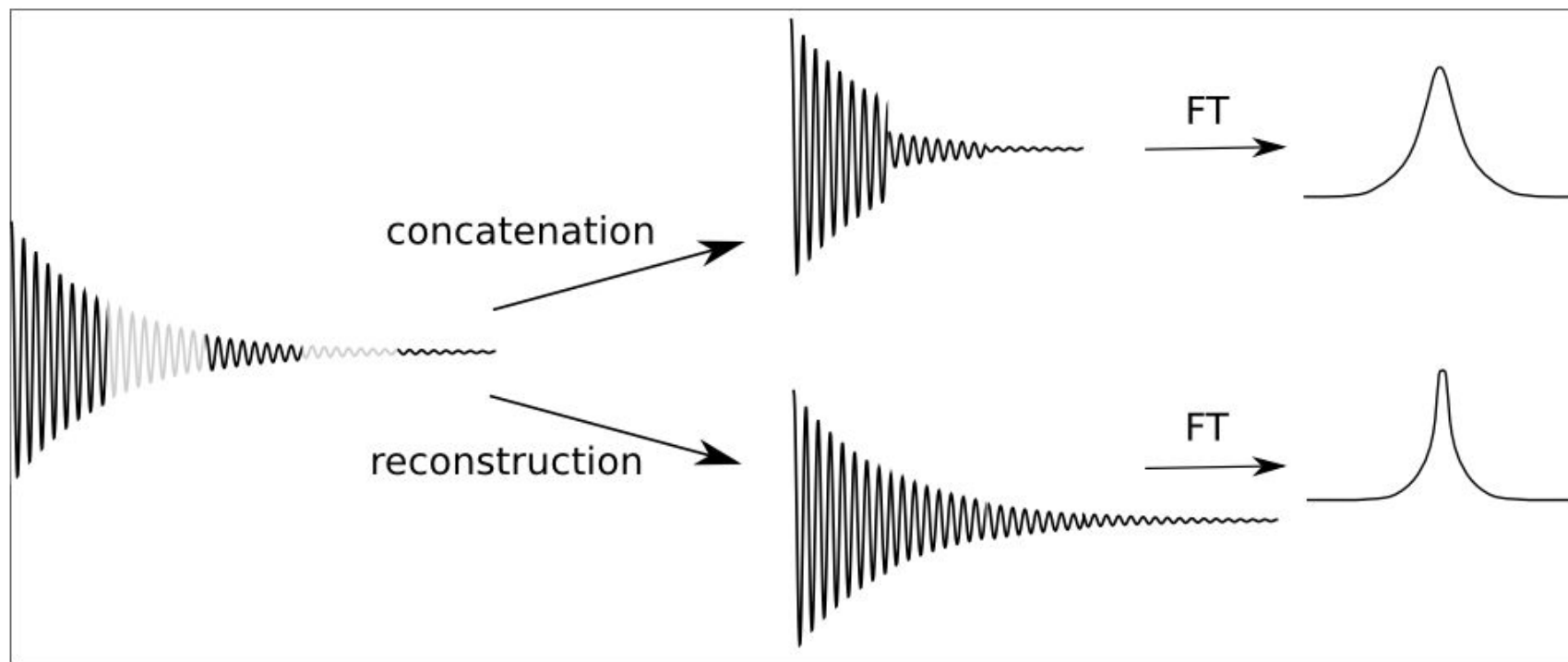
L. Castanar, T. Parella „Broadband ^1H homodecoupled NMR experiments: recent developments, methods and applications”, Magn. Reson. Chem. 2015, 53, 399–426

Pseudo-2D and real-time pure shift NMR



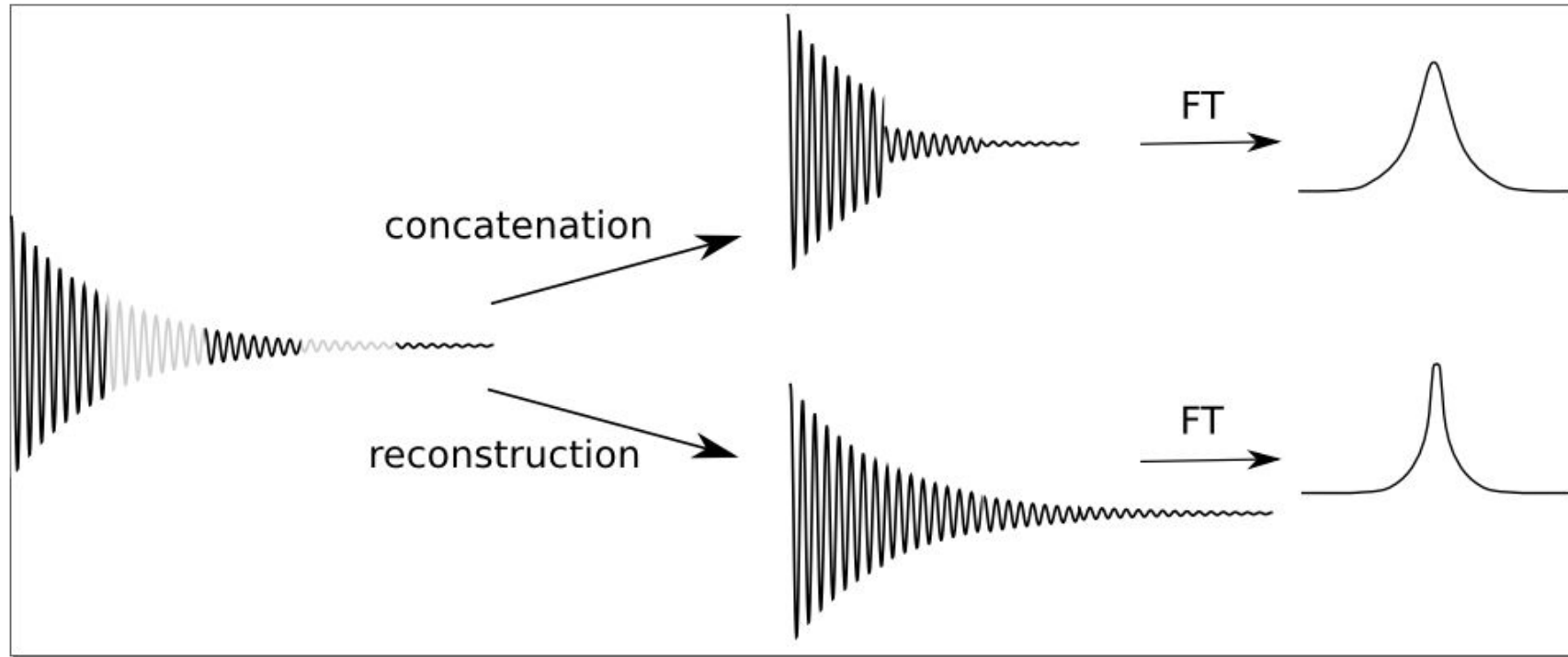
Real-time allows for „quick” measurements – suitable for e.g. unstable samples

Line broadening with concatenation



Line broadening with concatenation

Seemingly quicker relaxation with concatenation → need for reconstruction



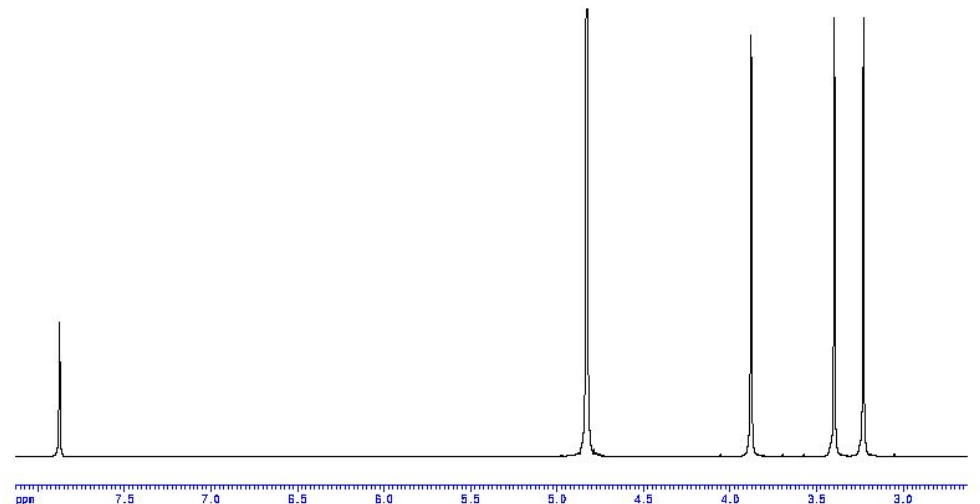
Compressed Sensing – basic idea

- A signal, which is **sparse** in some representation, can be undersampled (skip measurements) and then reconstructed mathematically

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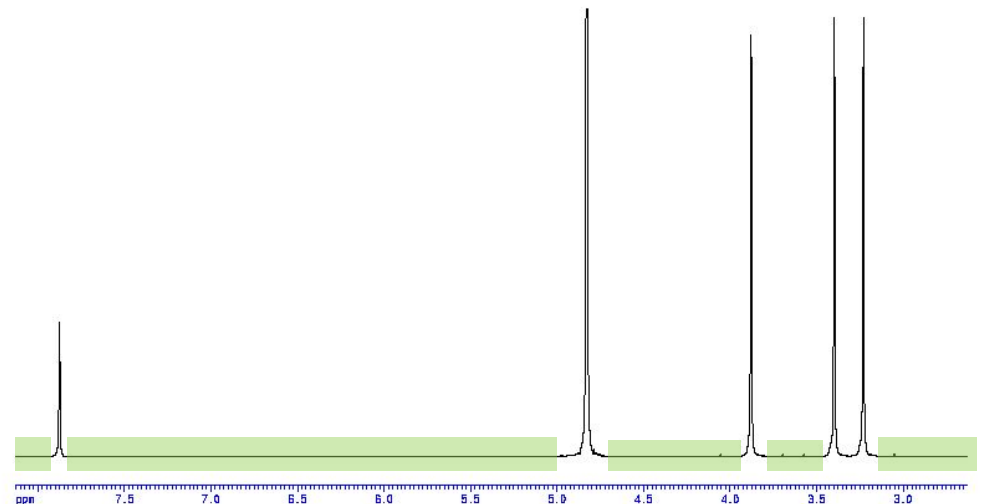
for NMR: spectrum
(Fourier transform of FID)



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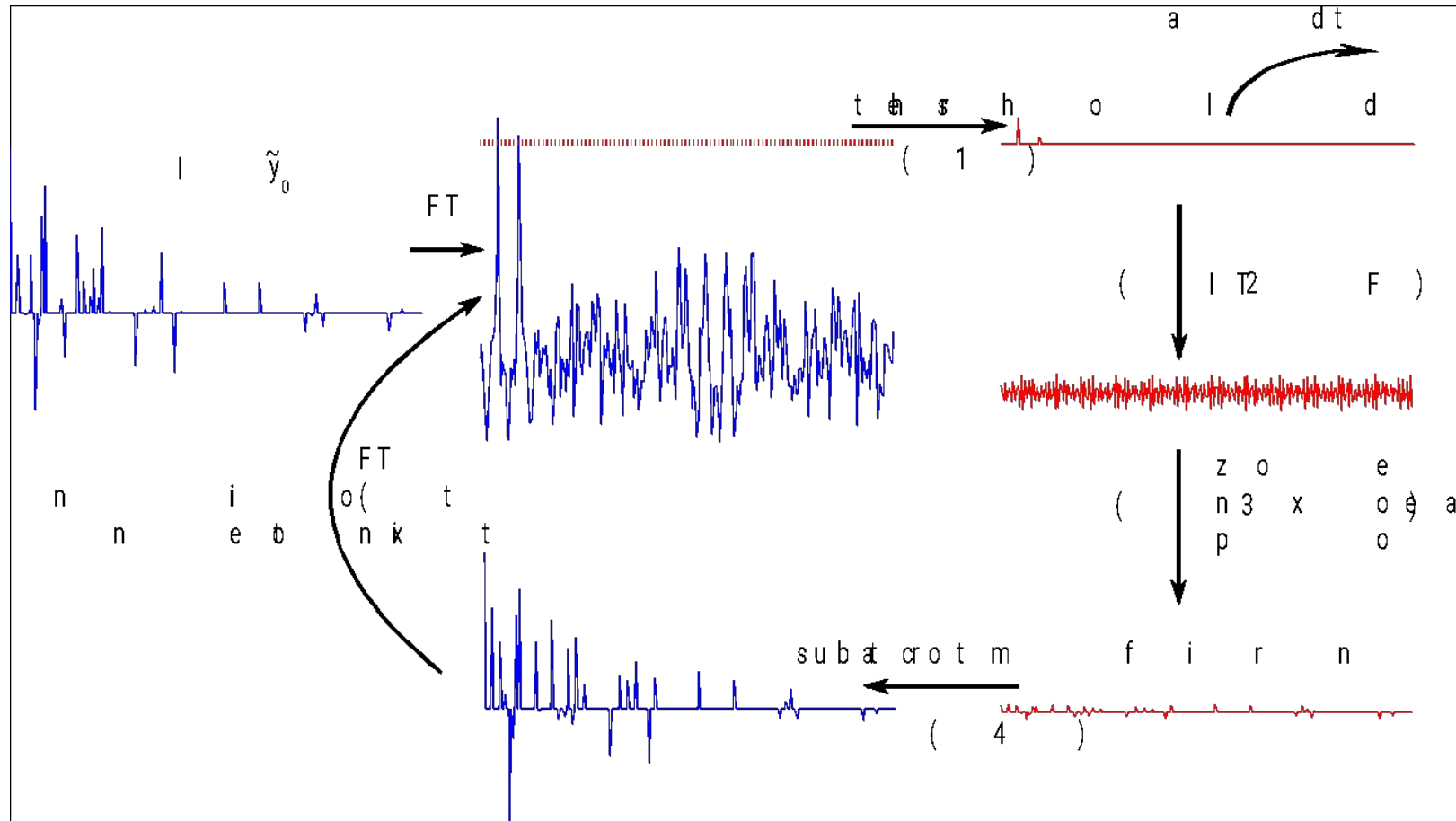
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- Iterative solution \rightarrow family of algorithms

Example – „Iterative soft thresholding”



Other applications

- Not only overcoming linebroadening in real-time pure shift experiments, but also:
- Safe extension of acquisition time while applying broadband decoupling (gaps in acquiring FID), with homodecoupling or without it



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CHEMPHYSCHEM
Communications

EXtended ACquisition Time (EXACT) NMR—A Case for 'Burst' Non-Uniform Sampling

Ikenna E. Ndukwe,^[a] Alexandra Shchukina,^[b, c] Krzysztof Kazimierczuk,^[b] Carlos Cobas,^[d] and Craig P. Butts^{*[a]}

- Safe fast-sampling techniques, e.g. ASAP sequences (submitted to ChemComm)

**Thank you
for you attention!**