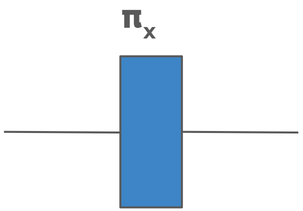
Composite Pulses

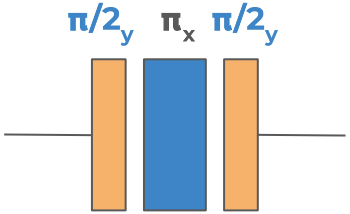
Overcoming Hard Pulse Limitations

Composite Pulses

- A composite pulse is simply **multiple hard pulses played back-to-back** to achieve the effect of a single excitation or refocusing pulse.
- A composite pulse is used to overcome limitations of single hard pulses, such as
  - **Sensitivity to pulse miscalibrations (B_1 sensitivity)**
  - **Offset dependence**
  - **Phase accumulation during excitation**



Hard π pulse

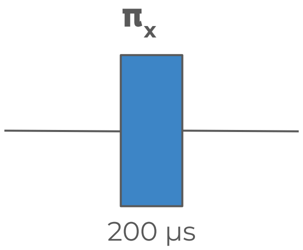


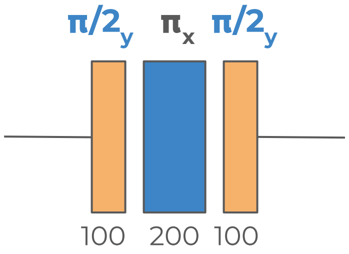
Composite π pulse (MLEV[1])

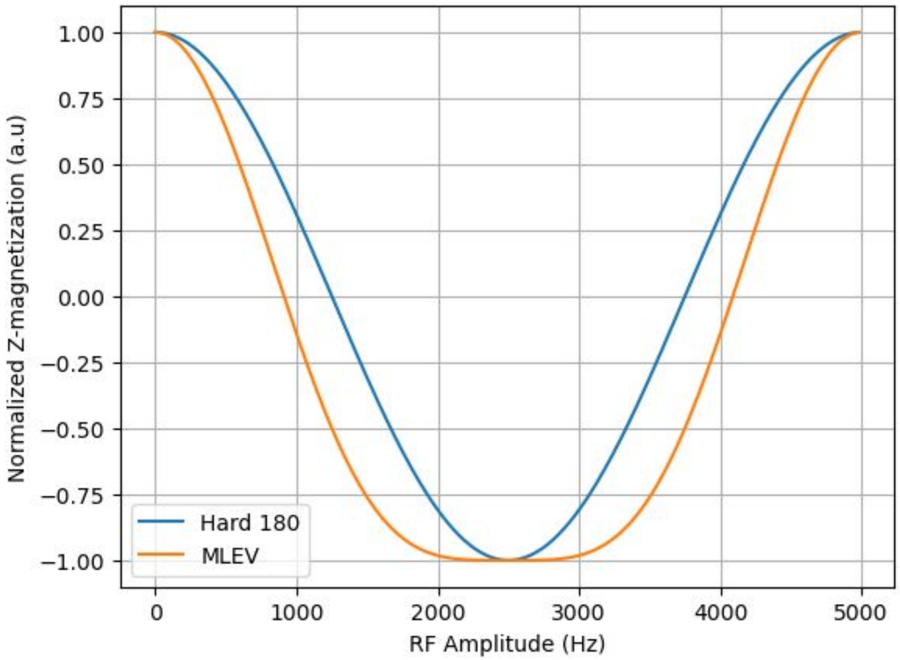
The **MLEV** composite pulse is one of the earliest & simplest composite pulses and widely used for inversion and refocusing.

1. Levitt, M. H., & Freeman, R. (1979). NMR population inversion using a composite pulse. *Journal of Magnetic Resonance (1969)*, *33*(2), 473-476.

Hard vs Composite Pulse: B_1 sensitivity

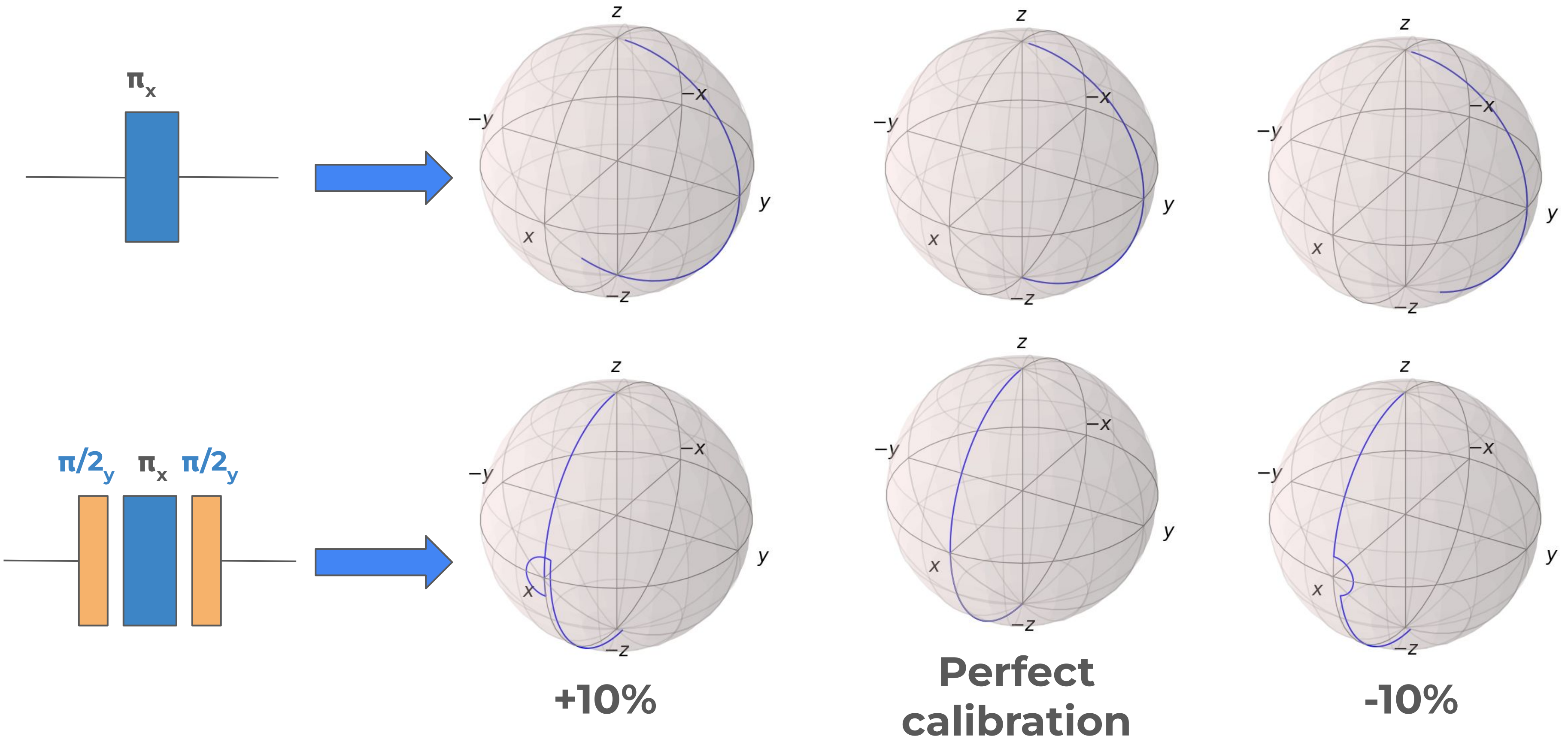






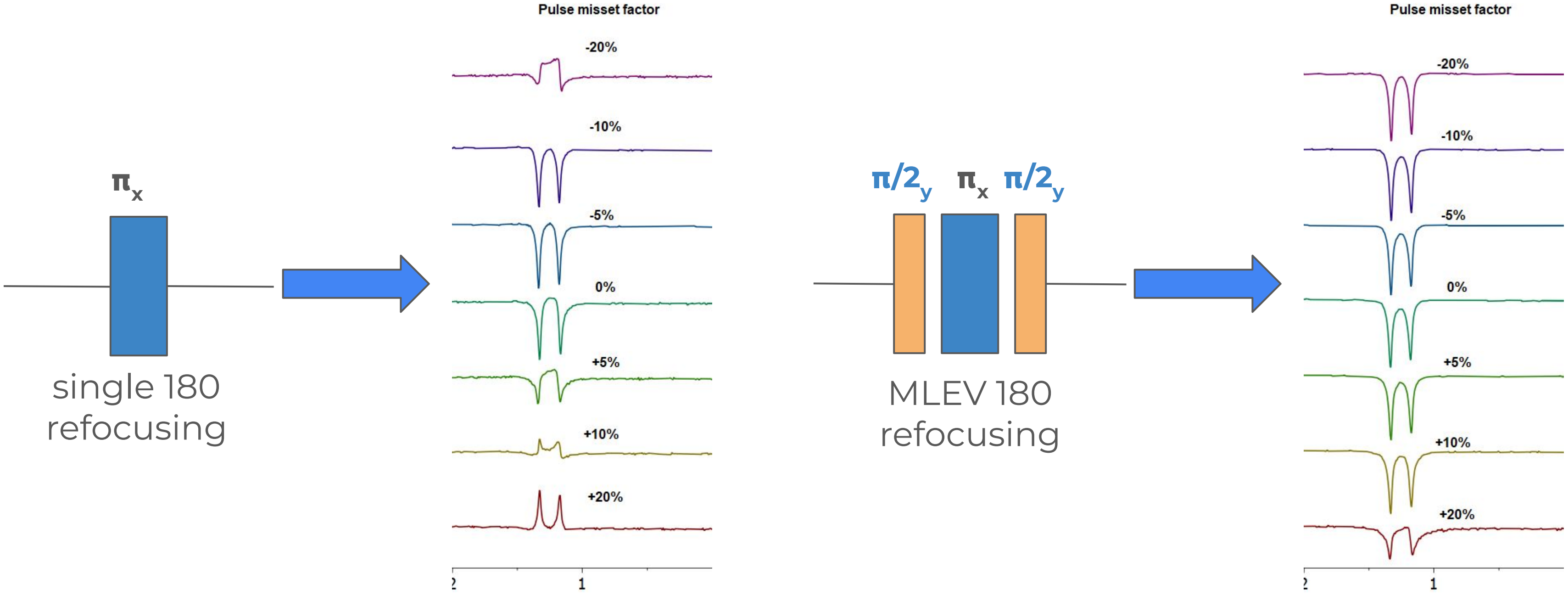
- This plot compares Z-magnetization (**M_z**) profile against pulse amplitude for a **200 μs hard** π inversion pulse vs a corresponding **MLEV** pulse.
- The optimal amplitude for complete inversion is 2.5 kHz, and for the **hard pulse**, any deviation from it results in **incomplete inversion.**
- However, **MLEV** can achieve **complete inversion** even if the amplitude is sub-optimal.

Magnetization trajectory when the inversion pulse power is off by ± 10%



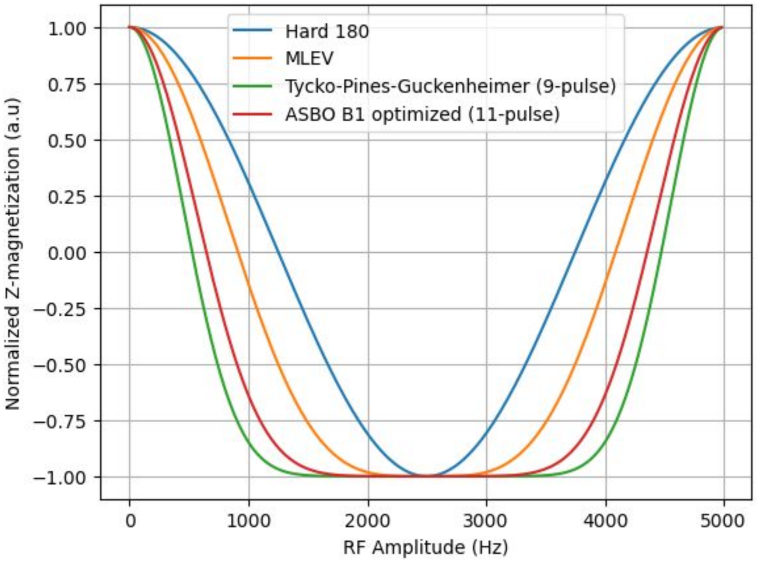
Example: CPMG Refocusing Pulses

CPMG experiments with a total **echo-time = 144 -ms**, using a **(1) single hard 180** and **(2) a MLEV 180** for refocusing, were performed on a sample of **lactic acid** in water. The echo-time was chosen such that the $-CH_3$ doublet is **inverted due to J-evolution**. It is clear that MLEV refocusing is much more resilient to pulse miscalibrations.



[Instrument info: Magritek Spinsolve, 1.04 T/**44.13 MHz** ^{1}H. Hard 180 calibrated at **32.4 us @ -2 dB**]

More B_1 insensitive composite pulses



- Over the years, various other composite pulses have been designed to compensate for pulse miscalibrations.
- Some involve as many as 13 hard-pulses.

Tycko-Pines-Guckenheimer anti-symmetric pulse[1]:

- Flip-angles: 180 ✖ 9
- Pulse Phases: **256 52 0 128 0 232 0 308 104**

ASBO-11 B_1 optimized anti-symmetric pulse[2]:

- Flip-angles: 180 ✖ 11
- Pulse Phases: **165 27.5 130 81.5 273 0 87 278.5 230 332.5 195**

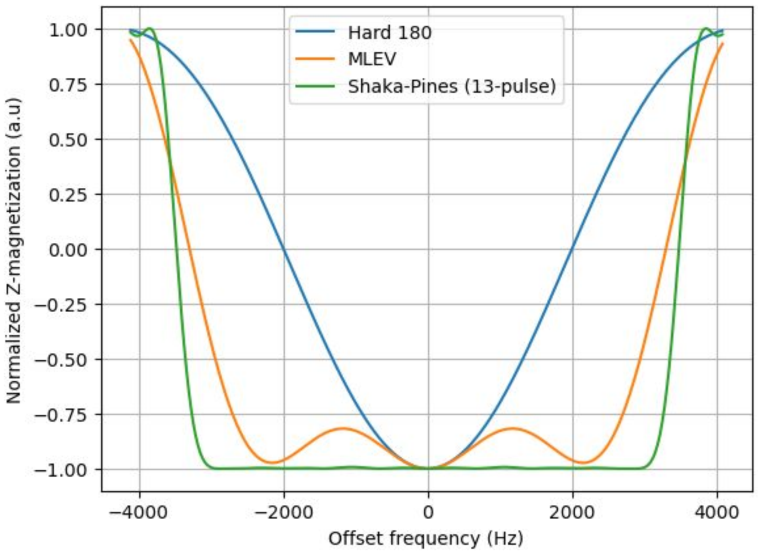
[Notice a pattern in the pulse phases?]

1. Tycko, R., Pines, A., & Guckenheimer, J. (1985). Fixed point theory of iterative excitation schemes in NMR. *The Journal of chemical physics*, *83*(6), 2775-2802.
2. Odedra, S., Thrippleton, M. J., & Wimperis, S. (2012). Dual-compensated antisymmetric composite refocusing pulses for NMR. *Journal of Magnetic Resonance*, *225*, 81-92.

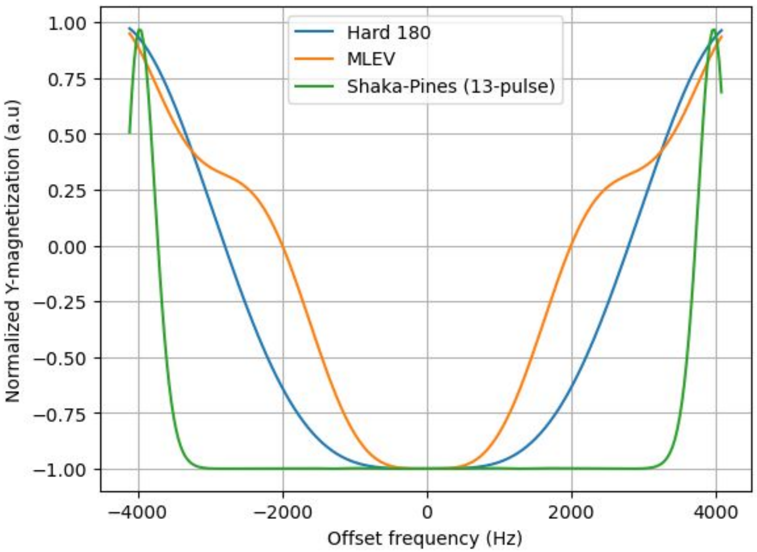
Offset independent Composite Pulses

Composite pulses can also be designed to achieve uniform inversion or refocusing over a given frequency range.

Inversion ($M_z \rightarrow -M_z$)



Refocusing($M_y \rightarrow -M_y$)



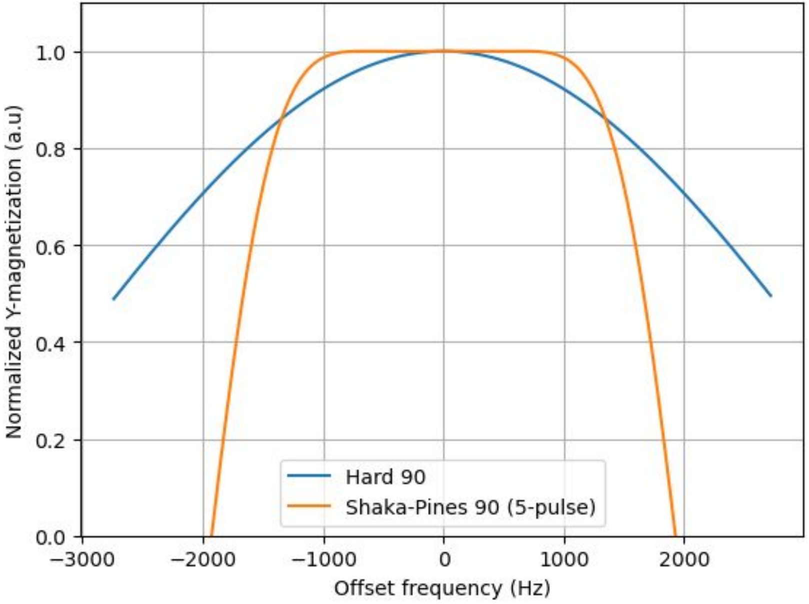
Shaka-Pines 13-pulse variant[1]:

- Flip-angles: **158 294 144 152 291 89 64 89 291 152 144 294 158**
- Pulse Phases: **0 180 0 180 0 180 0 180 0 180 0 180 0**

1. Shaka, A. J., & Pines, A. (1987). Symmetric phase-alternating composite pulses. *Journal of Magnetic Resonance (1969)*, *71*(3), 495-503.

Composite Excitation (90°)

Composite 90° pulses have also been designed to achieve **uniform, pure-phase*** excitation over a given bandwidth



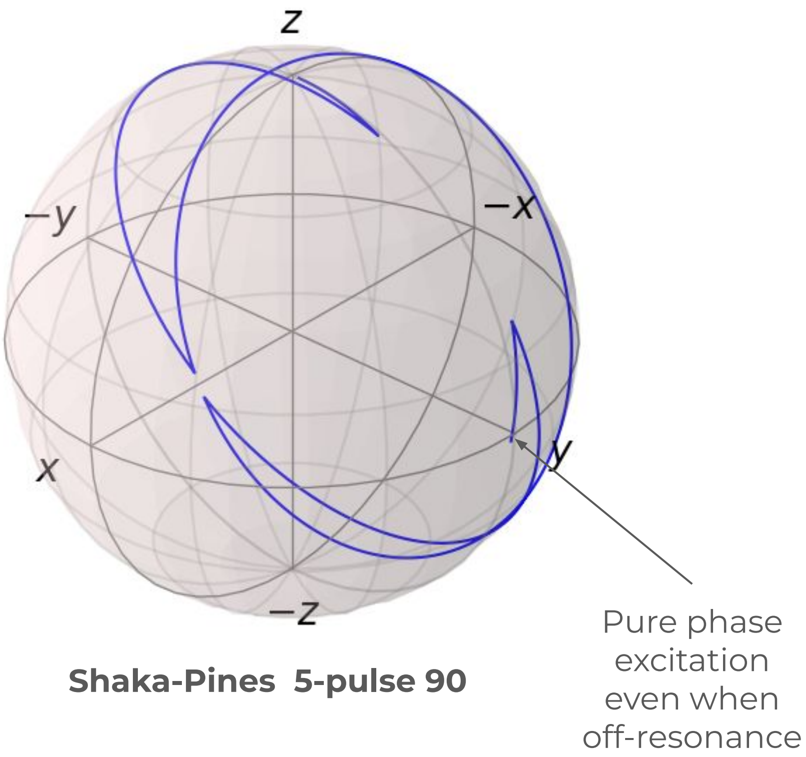
Shaka-Pines 5-pulse 90[1]:

- Flip-angles: **24 152 346 152 24**
- Pulse Phases: **0 180 0 180 0**

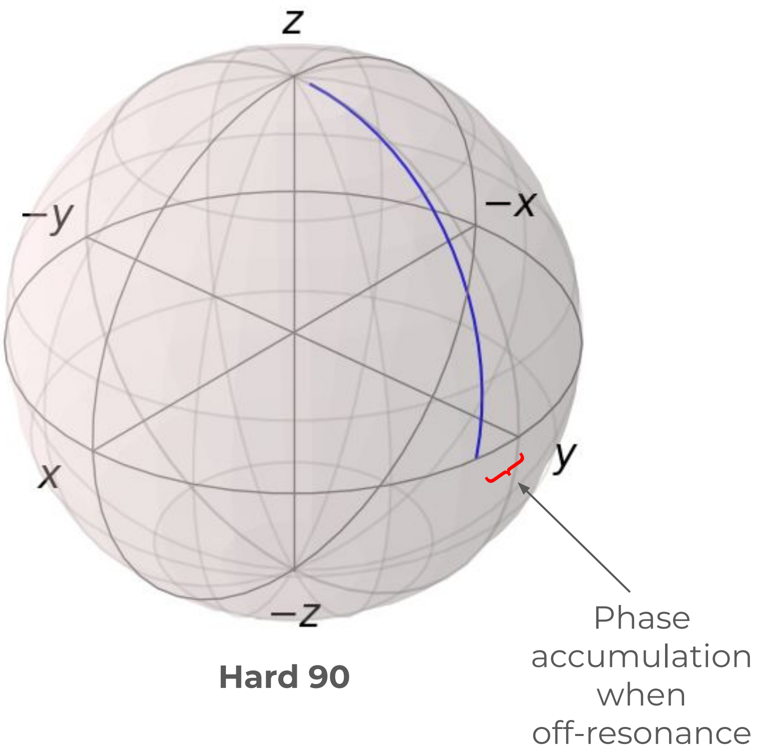
***pure-phase**: no phase accumulation during excitation, on $\mathbf{M_x}$ or $\mathbf{M_y}$ excited

1. Shaka, A. J., & Pines, A. (1987). Symmetric phase-alternating composite pulses. *Journal of Magnetic Resonance (1969)*, *71*(3), 495-503.

Magnetization trajectories at +500 Hz frequency offset



Shaka-Pines 5-pulse 90



Hard 90

In conclusion

- Composite pulses are a simple way to overcome limitations of single hard-pulses, especially for inversion and refocusing.
- Different composite pulses have been designed with different objectives:
  - **Insensitivity to pulse mis-calibrations**
  - **Uniform rotations across a wide bandwidth**
- The intended use determines which composite pulse to select.
- For robust inversion or refocusing, it is generally recommended to use a suitable composite pulse.
- Composite 90° pulses can also be used to achieve **uniform, pure-phase excitation without phase accumulation**.
- Recommended literature:
  - Levitt, M. H. (1986). Composite pulses. *Progress in Nuclear Magnetic Resonance Spectroscopy*, *18*(2), 61-122.