Shaped RF Pulses: Part 1

The Fundamentals

What are shaped RF pulses and why do we use them?

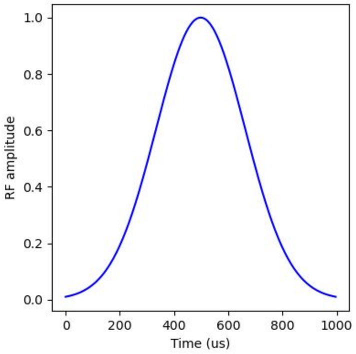
Certain NMR applications require **frequency selective pulses**:

- Solvent suppression
- Slice selection
- Selective excitation/refocusing of signals of interest

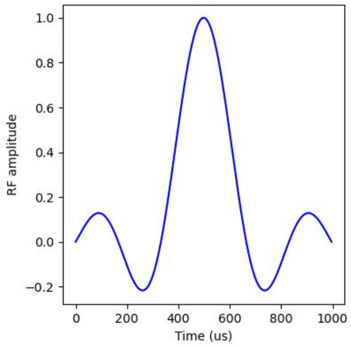
A **shaped pulse** is any RF pulse whose amplitude is modulated by some mathematical function or set of optimized parameters, designed such that it can **excite a well-defined range of frequencies**.

A few commonly used shaped pulses:

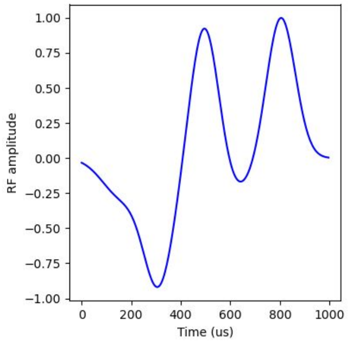
Gaussian



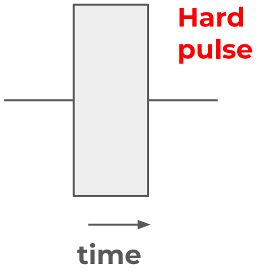
Sinc



Q5



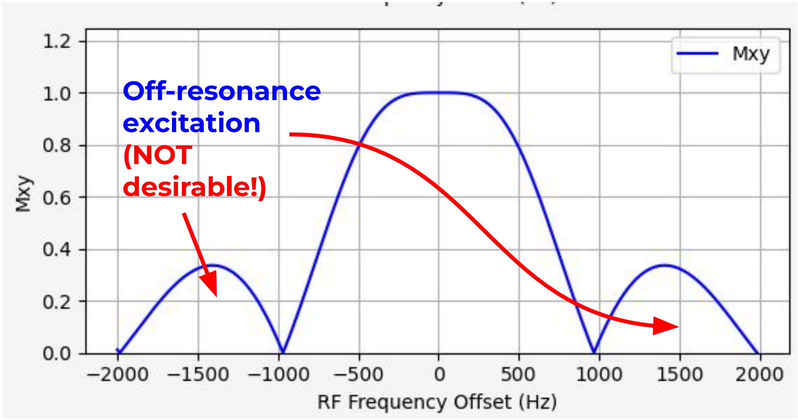
Why can’t we just use hard pulses?



(also called a ‘square’ or ‘rectangular’ pulse)

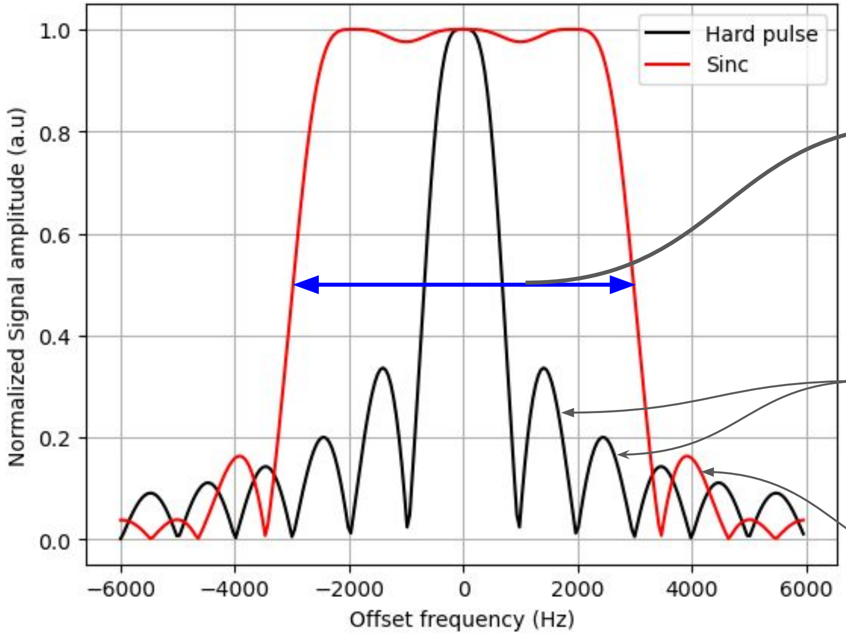
The **hard pulse** is the workhorse for NMR when **no frequency selective excitation** is needed. It is very poor at frequency selective excitation, with significant off-resonance excitation.

Excitation profile of a 1-ms Hard 90 deg. pulse:



What makes shaped pulses better?

Compare the excitation profile of a **1-ms Hard 90°** pulse Vs a **1-ms Sinc 90°** pulse:



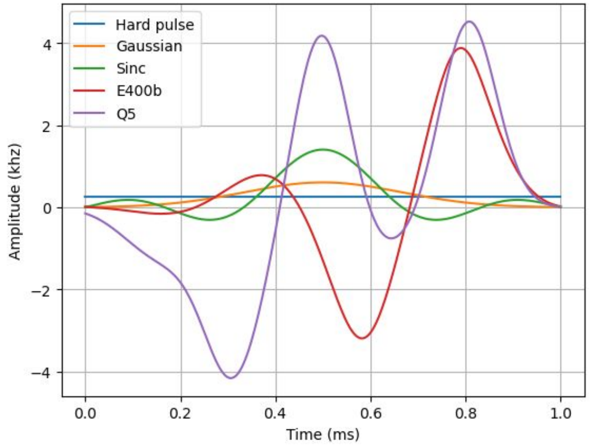
For the same pulse duration, the **Sinc** pulse provides a **far more uniform excitation** over a wider bandwidth.

These 'ripples' are undesirable!

(Sinc has these ripples too, but to a lesser extent)

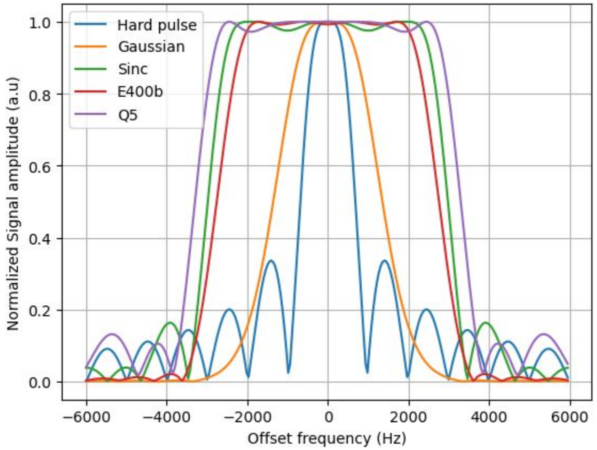
Let's compare a few different 1-ms shaped pulses

RF Shapes



Note that even though they are all the **same duration**, they have **different bandwidths**!

Excitation Profiles

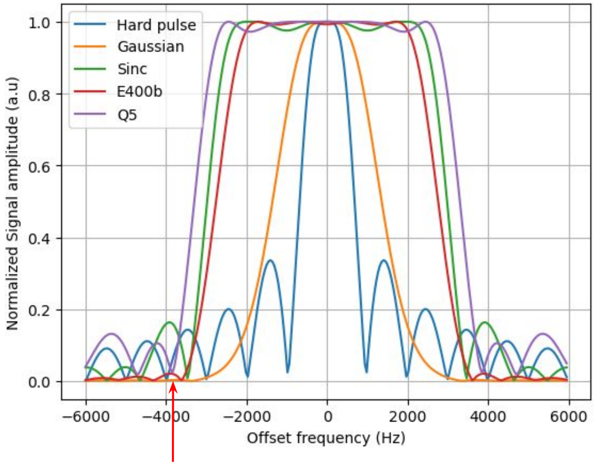


- Each unique shaped pulse is characterized by a constant: **Time-Bandwidth factor (R) = Pulse duration (ms) ✖ Bandwidth (kHz)** (Bandwidth being measured at the Full-width half-maximum of the frequency profile).
- For the same duration, a pulse with a **higher R**-value will excite a **larger bandwidth**.

Q5: Emsley, L., & Bodenhausen, G. (1992).Optimization of shaped selective pulses for NMR using a quaternion description of their overall propagators. *J. Mag. Res.* (1969), 97(1), 135–148.
E400b: Veshtort, M., & Griffin, R. G. (2004). High-Performance Selective Excitation Pulses for Solid- and Liquid-State NMR Spectroscopy. *ChemPhysChem*, 5(6), 834–850.

More on Excitation Profiles and R-value

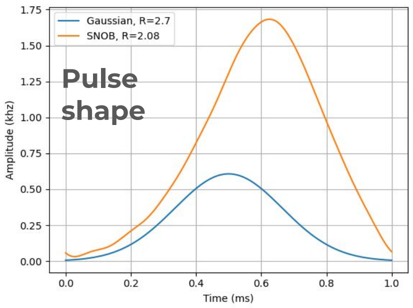
Excitation Profiles

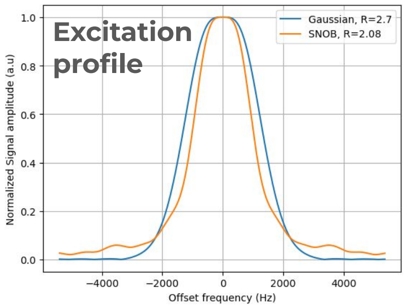


Note the minimal out-of-band ripples for E400b

- **Cleaner excitation profiles** are often achieved at the expense of **higher power requirements** (see Q5 and E400b on the previous slide).
- A **hard-90 has a R = 1.37**, while a **Gaussian 90** (truncated at 1%) has a **R = 2.7.** This means that a Gaussian will have almost double the bandwidth of a hard pulse for the same duration.
- The **R of a Sinc pulse can be approximated by the number of zero-crossings** (6 in the example here).
- Certain shaped pulses such as **SNOB** have been specifically designed to have a small R-value. This allows very narrow band excitation even with short pulses. **Gaussian** pulses are also good for this purpose.

Comparing **SNOB** and **Gaussian** pulses:

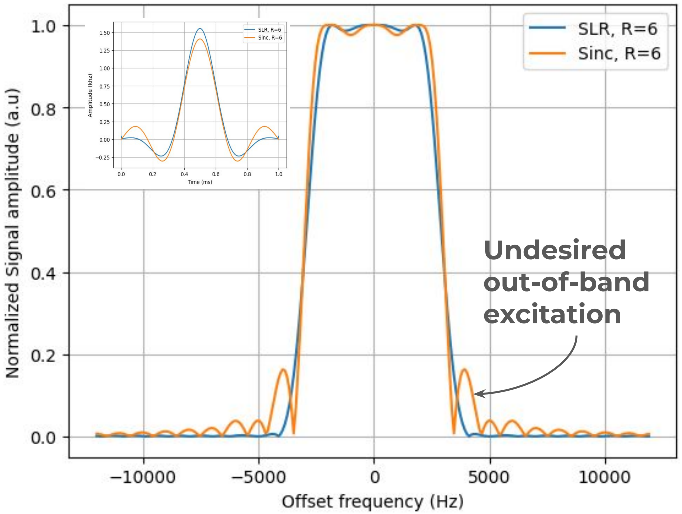




SNOB: Kupce, E., Boyd, J., & Campbell, I. D. (1995). Short selective pulses for biochemical applications. *Journal of Magnetic Resonance*, Series B, 106(3), 300-303.

Choosing shaped pulses

- The choice of shaped pulses depends on the use case. Some are suited for excitation, some are designed for inversion, while some are used exclusively for refocusing.
- **Low R-value** pulses (Gaussian, SNOB) are desired when only a **narrow frequency range** needs to be excited. Narrow-band excitation can be achieved by **high R-value** pulses as well, but require much **longer pulse duration**.
- For **uniform broadband excitation**, such as ultra-high field applications, **high R-value** pulses are desired.
- The ‘shape’ of the excitation profile is also critical, if the need is to **minimize** the effect on **out-of-band signals** (e.g. solvent suppression, where there are signals close to the solvent frequency)



Comparison of **1-ms Sinc vs SLR** pulse excitation profiles with **identical bandwidths**. The Sinc pulse will clearly have undesired effect on out-of band signals. The inset shows the pulse shapes.

SLR: J. Pauly, P. Le Roux, D. Nishimura and A. Macovski, "Parameter relations for the Shinnar-Le Roux selective excitation pulse design algorithm (NMR imaging)," in *IEEE Transactions on Medical Imaging*, vol. 10, no. 1, pp. 53-65, March 1991

In conclusion

- Shaped pulses play a very important role in modern NMR spectroscopy.
- There are numerous types of shaped pulses, each designed with specific properties to serve specific purposes.
- Knowledge of the excitation profiles of different shaped pulses allows us to choose the ones most suitable for our needs.
- Choice of pulses is often constrained by available RF power and maximum allowed power deposition.
- The advent of GHz-scale instruments has necessitated the design of new types of ultra-broadband pulses to uniformly excite the whole chemical shift range (at B_0 = 1 GHz, even 1-ppm ^{1}H is 1 kHz wide!). If interested, see publications from G. Veglia (U Minnesota) and B. Luy (Karlsruhe Institute of Technology).

Up next:

- Calculating shaped RF power,
- Composite pulses,
- Adiabatic pulses,
- Generating your own shaped pulses from Fourier coefficients,

and more...

Recommended resources to learn more about shaped pulses

- Robin de Graaf, *In vivo NMR Spectroscopy: Principles and Techniques*, 3rd Edition
- Timothy Claridge, *High-Resolution NMR Techniques in Organic Chemistry*, 3rd Edition