Journal of Magnetic Resonance Open 10-11 (2022) 100026

Contents lists available at ScienceDirect

Journal of Magnetic Resonance Open

journal homepage: www.sciencedirect.com/journal/journal-of-magnetic-resonance-open

# Mechanism of chirp excitation

Sreya Das, Justin Jacob, Navin Khaneja *

System and Control Engineering, IIT Bombay, Powai 400076, India

ABSTRACT

In design of a chirp inversion pulse, we keep the sweep rate $a \ll \omega_1^2$, where $\omega_1$ is the amplitude of the pulse. This is the adiabaticity condition for the inversion to work. We can convert a chirp inversion pulse to an excitation pulse by keeping the chirp rate high, with $a > \omega_1^2$. To be precise $a = 2.8\omega_1^2$. The analysis of such a pulse breaks the evolution into three phases. The first and third phase are adiabatic phases while the second phase is non-adiabatic. Starting from north pole such a pulse brings the magnetization to equator, however there is a nonuniform phase which depends on the resonance offsets. We show how by following this pulse with a chirp inversion pulse at twice the sweep rate of excitation pulse, we can refocus this uniform phase. We find there is still some phase dispersion. This can be further eliminated by bringing in a second inversion pulse. The combination of these three chirp pulses allows us to excite arbitrary large bandwidth without increasing the peak amplitude of the pulse. Refocusing properties of pair of chirp has been studied before but our description is very different.

## 1. Introduction

Broadband excitation is a fundamental problem in NMR spectroscopy. The goal is to excite magnetization with resonance offsets lying a certain spectral range due to phenomenon of chemical shifts. Higher spectrometer field strengths provide significantly increased sensitivity and spectral resolution, but the sample must also be excited over a correspondingly expanded range of chemical shift frequencies. Ideally, one would like the excitation profile over the range to be uniform, producing transverse magnetization of constant phase. Keeping pace with steadily increasing field strength is a challenge, given maximum power tolerances of typical RF probes. At a field of 1 GHz, the target bandwidth is 50 kHz for excitation of entire 200 ppm $^{13}$C chemical shifts. The required 25 kHz hard pulse exceeds the capabilities of most $^{13}$C probes and poses additional problems in phasing the spectra. In $^{19}$F NMR, chemical shifts can range over 600 ppm, which requires excitation of different regions of the spectra. Methods that can achieve uniform excitation over the entire bandwidth in $^{19}$F NMR, are therefore most desirable. Towards this end, several methods have been developed for broadband excitation/inversion, which have reduced the phase variation of the excited magnetization as a function of the resonance offset. These include composite pulses, adiabatic sequences, polychromatic sequences, phase alternating pulse sequences, optimal control pulse design, and method of multiple frames, [1–12,14–32].

In this paper we study a broadband adiabatic pulse, *Chorus* [26] which gives uniform excitation over unprecedented frequency range, with a uniform phase. *Chorus* is a composite adiabatic pulse. It has a pulse element that produces excitation of magnetization we call it chirp excitation. In this paper, we elucidate the mechanism behind working of chirp excitation [13]. We first develop a three stage model for understanding chirp excitation in NMR. The phase of magnetization resulting from chirp excitation pulse is non-uniform as function of offsets. We then show how a chirp $\pi$ pulse can be used to refocus the phase of the excitation pulse. The resulting magnetization still has some phase dispersion in it. We show how a combination of two chirp $\pi$ pulses instead of one can be used to eliminate this dispersion leaving behind a small residual phase dispersion. The pulse sequence presented here allows exciting arbitrary large bandwidths without increasing the peak rf-amplitude. Although methods presented in this paper have appeared elsewhere [3,5,26,32], we present complete analytical treatment that elucidates the working of these methods. The paper further develops the treatment in [13] by providing more elaborate and transparent proofs.

The paper is organized as follows. In Section 2, we present the mechanism behind chirp excitation. In Section 3, we present simulation and experimental results for broadband excitation pulses designed using chirp pulses. We conclude in Section 4, with discussion and outlook.

## 2. Theory

Let

$$\Omega_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \; \Omega_y = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \; \Omega_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

* Corresponding author.
*E-mail address:* nkhaneja@sc.iitb.ac.in (N. Khaneja).

https://doi.org/10.1016/j.jmro.2021.100026
Received 4 September 2021; Received in revised form 3 December 2021; Accepted 7 December 2021
Available online 9 December 2021