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Reply on RC2

Jens D. Haller et al.

Author comment on "SORDOR pulses: expansion of the Böhlen–Bodenhausen scheme for low-power broadband magnetic resonance" by Jens D. Haller et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-1-AC2, 2022

Dear Referee #2,

We also thank you very much for your knowledgeable comments, which certainly improved the readability of the manuscript significantly, particularly to readers that are less familiar with the details of pulse design. Please find the specific replies to your comments below. We very much hope that with the changes made you will agree to publishing the revised version of the manuscript.

Sincerely yours,

Jens D. Haller, David. L. Goodwin, Burkhard Luy

In this manuscript, Haller et al. describe a possible application of a recently reported class of radio-frequency pulses to low-power broadband NMR. The SORDOR pulses were designed with optimal-control theory to achieve universal rotation by 90° or 180° and a quadratic offset dependence of the phase. In this work combination or SORDOR pulses are used, with a specific example given for the case of the PROJECT pulses sequence. The idea of using OC-derived pulses for low power broadband MR, and, e.g., allow for broadband mixing, is interesting and useful. The reported experimental data is also well presented. However, several aspects of the theory and simulation are very difficult to follow for the non-expert reader. I recommend addressing the following issues before the paper can be considered for publication. They mainly consist in giving more background for the key concepts and results, and stating the main conclusions of the paper much earlier.

Throughout the paper, reference is made to the Böhlen-Bodenhausen scheme. It would be useful to explain what this actually is. My expectation was that this phrase referred to the use of combinations of frequency modulated pulses to remove the non-linear offset dependence of the phase that arise when using just one (the first paper by Böhlen and Bodenhausen). But the authors specifically do not show this. So what it the Böhlen-Bodenhausen scheme ? Using combination of frequency swept pulses ? Or is there some specific combination that should be met ?

In the same line, it might be useful to name the method with a phrase that describe what it does, rather than the name of those who first described it (especially since they described several different things).

>>> Böhlen and Bodenhausen published several different refocusing approaches based on linearly frequency-swept adiabatic pulses that result in quadratic phase behavior with respect to offset (as the phase is the first derivative of the frequency with time). We call the sum of all these refocusing approaches based on quadratic phase pulses the Böhlen-Bodenhausen concept. We explain this now in more detail in the introduction.

The authors write "the quadratic phase correction of the acquired FID may be compensated by using a SORDOR-180 pulse with twice the rf-amplitude and half the pulse length tp for refocusing. In this case the frequency sweep is twice as fast as for the nominal SORDOR pulses and the quadratic phase should fully refocus to a normally phased spectrum." Considering the relevance of having directly phasable spectra, the authors should demonstrate this experimentally…

>>> We had a close look at the compensation of the quadratic phase. It turns out that ideal conditions are obtained with a SORDOR-180 pulse with rf-amplitude and pulse length scaled by square-root 2. As a result, no phase correction is needed with this type of refocusing before acquisition. We demonstrate the approach experimentally in new Figure 4 and changed/added to the text accordingly.

… especially since the introduction states "if a simple quadratic phase correction of the spectra can be tolerated". In which cases is there a solution if it cannot be tolerated ?

>>> We reformulated the sentence. In some cases quadratic phase corrections might lead to spectral artefacts. For example, if a very broad background is present in a spectrum a quadratic phase correction might result in a wavy baseline. But with the refocusing using the scaled SORDOR-180 pulse the quadratic phase correction can be avoided, circumventing also the background problem.

One of the main point seems to be that SORDOR pulses achieve universal rotation, which classic chirp pulses do not. Figure 1 illustrates this, but it is difficult to follow without a more detailed description of what "effective rotation" means, and what the different frames are (x, y, z) and (X, Y, Z). Please give more background information.

>>> We apologize for the confusion caused by using lower-case (x,y,z) in the main text and upper-case (X,Y,Z) in Figure 1. The coordinates in both cases refer to the rotating frame. We have changed Figure 1 to now include also lower-case (x,y,z). The effective rotation of a shaped pulse consisting of n piecewise constant individual pulses is defined via its effective propagator $U_{eff} = U_n \dots U_1$, which for a single spin ½ represents a simple effective rotation in 3D space. We added the mathematical definition with a comment in the theory section.

It is known that linearly frequency swept pulses with gamma B1 / (2pi) = sqrt(BW/Tp) achieve uniform 90° excitation (see Tal and Frydman, Prog. Nucl. Magn. Reson. Spectrosc. 2010), with a quadratic dependence of the phase. How can this be reconciled with Fig. 1? And with the statement "it is obvious that the adiabatic pulse can only used to excite a single component". Addressing these two questions and the previous one would help (the non expert reader) to understand what is it that can be done with SORDOR pulses and not chirp pulses.

>>> First, the authors would like to make the statement of the referee more precise: linearly swept pulses (under certain conditions) achieve uniform excitation with an effective 90° flip angle starting form z-magnetization. The original z-magnetization is then distributed in the transverse plane with a quadratic dependence of the resulting x,y-phase with respect to the offset. A "uniform 90° excitation" as stated by the referee is therefore NOT a universal 90° rotation (UR90)! The effective flip-angles of initial x- or y-magnetization may and will deviate considerably from 90°! Only a single component, the initial z-magnetization, experiences a "uniform 90° excitation". It is therefore a classical PP (point-to-point) pulse with a quadratic phase behaviour. It is NOT a B1 class pulse with a pi/2 effective rotation in the x,y-plane.
SORDOR-90 pulses, on the other hand, are B1 class pulses and 90° mixing like in a COSY experiment can directly be implemented without additional refocusing. Next to a clarification in lines 33-38 (see below) we also introduced an explaining sentence in the conclusion.

Looking at Fig. S1, the difference between SORDOR and chirp pulses seems to be significant mostly for 90° pulses. It is stated in the conclusion but it would help if it were stated much earlier. It would be interesting to rearrange Fig. S1 so that it can be included as Fig. 1.

>>> We rearranged the previous Fig. S1 to be the new Fig. 1. We state in the main text close to Fig. 1 regarding the similarity of SORDOR-180 and CA-Chirp-inv pulses: The SORDOR-180 pulse shows the very same rotation behaviour as the SORDOR-90 pulse, just with an effective 180° rotation angle in the x,y-plane throughout the optimised offset range. As such it resembles very much the behaviour of the CA-Chirp-inv pulse of same duration and rf-amplitude. However, the SORDOR-180 pulse is directly matched in its phase behaviour to the SORDOR-90 pulse, which for an adiabatic inversion pulse would only accidentally be the case.

It would help to address all of the above if l. 33-38 could be rewritten in more details:. what does "matching pulse shapes" mean ?
. "the inversion pulses acts as a refocusing […]"; how is that a consequence of the fact that "the effective phases of the pulses are matched"
. "Matching UR-90 pulses, however, […]"; this sentence seems to be the key part of the paper but it is difficult to understand.
. the explanation on COOP pulses is confusing, as it mentions "the least amount of restrictions" and then "similar restrictions".

>>> We have rewritten and extended lines 33-38 and the following paragraph to explain in more detail the matching of the pulse shapes: "Depending on the offset ω_z, adiabatic excitation transforms z-magnetization into transverse magnetization with pulse-dependent phase angles $\alpha(\omega_z)$ with respect to the x-axis. A following matched adiabatic inversion pulse provides an effective rotation around the phase $\alpha(\omega_z)+\varphi$ with either constant or linearly offset-dependent phase φ. As the effective pulse phases are matched in this concept, the inversion pulses act as refocusing (UR-180) pulses with a quadratic offset dependence of the corresponding rotation axes, where the quadratic phase originates from the linear frequency sweeps of the adiabatic pulses. A more general concept without the restriction to linear frequency sweeps is the COOP concept introduced by Braun and Glaser. But also here excitation pulse shapes introduced so far are PP pulses, resulting in limited applicability."

The author could define, maybe in the SI, what the “pulse performance” and “quality factor” are.

>>> (theoretical) pulse performance and quality factor have been used as synonyms, both referring to Phi as defined in new equation (1). We have added Phi to “pulse performance Phi” or “quality factor Phi” at several positions in the text for more clarity.

A comment following the posting or review 1: I entirely agree with reviewer 1 that the citation styles makes some parts of the manuscript very difficult to read. It would be much preferable to use numbered references.

>>> As this subject is a matter of taste, we leave any format change applied to the editors.