

Interactive comment on “Heteronuclear and Homonuclear Finite Pulse Radio Frequency Driven Recoupling” by Evgeny Nimerovsky et al.

Anonymous Referee #3

Received and published: 4 January 2021

This manuscript presents an operator analysis of the well-known fp-RFDR recoupling sequence with some emphasis on the XY phase cycling scheme. The benefit of this analysis should have been defined at the end of the introduction.

Allow me to make some comments on the text:

115: What is meant here by an analytical integration?

120,146: “by I3 spin system”. Please define this system- “by THE/A I3 spin system”.

130: what is the definition of f in $f \in \text{f} \text{A} \text{ö} \text{CSA}, 2$.

147,155: sum over $r < s = 1, 2, 3$? and add a dot between I_r and I_s .

152: If the model Hamiltonian provides an equivalent spin evolution as of the full Hamil-

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tonian at specific time points, then there are two possibilities. If the specific points are equally spaced in time, I would call it an average Hamiltonian. If they are not equally spaced in time, then I do not see the purpose of introducing a “model” Hamiltonian. I can appreciate the fact that the average Hamiltonian can be derived not theoretically but numerically, but then it should be general enough, in terms of variations of the spin parameters, to be significant.

164: That the red and black lines cross each other is not a surprise. If the amplitudes of all operators would cross the corresponding black operators at the same equally spaced positions then we can think about an average Hamiltonian.

— 194: Would the result at this point mean that the three model Hamiltonians in Eq. (2) are not adequate to provide a general form of the average Hamiltonian?

213: That the secular Hamiltonian plays a significant role in the transfer is not really a surprise. Without this part of the Hamiltonian there would be no dipolar interaction. The flip-flop terms can be (partially) quenched because of off-resonance effects, thus the conclusions on the top of page 11 are surprising. They are however not very practical when dealing with CSA tensors in rotating samples where the frequency differences are modulated by the spinning. Therefore, there seems not to be a clear conclusion about the choice of the three model Hamiltonians and in the rest of the manuscript, the full Hamiltonian is applied in all cases.

When dealing with the IS spin system it should be stated from the beginning that the fp-RFDR sequence looks like Fig. 10.

224: The “same” value of the dipolar interaction strength results for a homo-nuclear spin pair in a static spectral line splitting that is 50% larger than for a hetero-nuclear spin pair. Thus, only when spectral frequencies are considered and for “display reasons” their values are compared, it is practical to increase the hetero-interaction artificially by a factor of 1.5. In MAS one should be careful doing so, because the sideband patterns are not straightforwardly showing this 1.5 spectral factor.

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238–: What is the purpose of the extended analysis of all 14 operators as a function of offset. What do they tell us? Here again it would have been nice to know what the aim of this part of the study is. From the experimental point of view, what is of interest is the operator that results in the signal. That particular operator should have been emphasized. The study does not tell us about the yield of polarization transfer. Following the text following page 11, much details are presented and it is hard to follow the main line of thought. Perhaps summarizing the conclusions, followed by some examples (and moving part of the figures to a supplementary file), would help the reader to comprehend what is going on. Also the effects/benefits of the XY phase cycling should be characterized separately from the corent pathways.

416 –: If part of the numerical derivations are intended to introduce the yield of the hetero-nuclear polarization transfer experiments, then that should have been stated from the beginning. Here again the various comparisons between the experimental spectra are a bit confusing. Perhaps some consistent conclusions at the end of page 22 can form a basis for the analysis of the spectra.

Interactive comment on Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2020-30>, 2020.

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