

Interactive comment on "Origin of the Residual Linewidth Under FSLG-Based Homonuclear Decoupling in MAS Solid-State NMR" by Johannes Hellwagner et al.

Malcolm Levitt (Referee)

malcolmhlevitt@mac.com

Received and published: 29 December 2019

This is a very detailed and authoritative study of the origin of residual linewidth in magic-angle-spinning FSLG proton NMR experiments. The paper contains state-of-the-art theoretical derivations (based on Floquet theory) and numerical simulations to elucidate the issue. The paper also contains results of attempts to compensate for pulse phase transients using amplitude modulation of the radiofrequency fields.

Despite the very high quality of this work I found a few issues not completely clear and propose that they should be corrected before acceptance.

C1

1. The abstract mentions "static rf-field inhomogeneity". This might be a simple typo. I do not know what a "static rf field" is.

2. Figure 1 compares analytical and numerical simulations of several three-spin tensor operators that may contribute to residual linewidths. However it is not very obvious, neither in the figure annotations, nor the captions, what the definitions of these operators are. This also applies to the text. For example at the top of page 7, an operator $T_{00}(\tan_4)$ is specified but it is unclear to me what \tan_4 is. Maybe I missed something but I don't find the definition or relevance of \tan_4 . Similar problems occur in many places. The authors should give clear definitions (if necessary, in the SI, or literature references) for all the terms mentioned in the paper.

3. One point I would like clarifying is whether the only type of rf field imperfection that was considered was (possibly transient) errors in the rf amplitude. I am aware of two other imperfections that deserve consideration. First, phase errors are generated by a limited bandwidth probe when the input frequency is changed (as happens in a FSLG experiment). Early implementations of this method did use a relative phase adjustment of the two pulses to correct this effect (see http://www.sciencedirect.com/science/article/pii/B9780120255146500113). I wonder whether the more modern compensation algorithms already include such a phase correction (it is possible that this is so, but clarification is needed). The second feasible error is that spatial inhomogeneity in the direction of the radiofrequency field causes a periodic phase modulation as the sample rotates. NMR effects due to this have been detected in rotary resonance experiments (http://onlinelibrary.wiley.com/doi/10.1002/ijch.198800039/abstract). It is possible that such effects might also contribute to the residual linewidths.

Apart from these minor issues the paper is of excellent quality and high importance to the field and should be published after minor revisions.

Interactive comment on Magn. Reson. Discuss., https://doi.org/10.5194/mr-2019-5, 2019.