

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

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I agree with Malcolm and the 2nd referee on the overall quality of the manuscript. I just had a few comments on making the presentation more accessible for the non-expert and putting the work in wider context.

One aspect that didn't come across clearly was which spin parameters were significant in the third order terms, particularly in section 4 where heteronuclear couplings are now involved. Various spin operators are quoted, but it is not always clear whether these cross terms are arising from homonuclear dipolar couplings or heteronuclear dipolar couplings, cross-terms with offsets (or even 1H CSA). The analytical section

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refers to multiple three-spin operators, but presumably not all the contributions to the 3rd order terms will involve 3 spins? Hence, I found the discussion on P10 and P11 a bit confusing. What exactly is meant by "simulations with one and two dipolar couplings", a CH vs. a CH₂ spin system or is it H₃? Similarly, I had to read the caption of Fig 4 a couple of times, e.g. (A) and (B) are showing calculated splittings, rather than "simulations" or "Full scale linewidths". It would be better to say "without taking chemical-shift *scaling* into account" ("correction" is a bit vague and could refer to referencing).

Is Fig. 7 is showing ¹³C or ¹H T₂'? The sudden shift to heteronuclear systems is a little jarring. In this context, I must disagree with the characterisation in the introduction of our work on 3rd order contribution in heteronuclear systems (Tatton, 2012) as merely "qualitative"! There was greater emphasis on numerical simulation; analysis was confined to the simple LG, with the merit that simple expressions could be obtained for the 3rd order contributions, but it was certainly quantitative, and considered some of the same problems (influence of ¹³C heteronuclear couplings on ¹H homonuclear decoupled spectra). So the two papers are nicely complementary; indeed the contribution of ~60 Hz to the linewidth agrees well with the earlier work, not just Fig S2!

Figure 8: Is a pi pulse being used in experimental spectra to refocus shift evolution in the indirect dimension? Were the simulations of the full 2D experiment or a 1D version? It will not affect the conclusions, but you wouldn't experiment the two versions of the experiment to match up quantitatively.

Minor detail: Methanol and Ethanol in Materials and Methods should be lower case.

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