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A few additional comments

Stefan Stoll (Editor)

Editor comment on "Intermolecular contributions, filtration effects and signal composition of SIFTER (single-frequency technique for refocusing)" by Agathe Vanas et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-17-EC2, 2022

In addition to the reviewers'comments, I am adding a few remarks as well:

This is an interesting paper that adds theoretical insight about how dividing a SIFTER signal by a SIFTER signal without the second pi/2 pulse--called SIDRE here--is valid for removing unmodulated signal contributions.

[1]
The main practical implication of this work is that the signal division approach is valid. This should be emphasized more.

[2]
This division approach is not new. It was first proposed and succesfully utilized in Spindler et al, J.Magn.Reson. 280, 30 (2017), see Fig. 6 and discussion at the end of section 3.5 around eq.7. The authors do not cite nor disucss this originial prior work. This references should be cited, alongside the similarly early and relevant 2017 Denysenkov reference and the 2018 Bowen reference, in a prominent place such as the introduction.

[3]
The entire Section 2 is very difficult to follow, due to notational inconsistencies and omissions, combined with a verbose and at times meandering narrative. It's all probably rigorous and correct, but it is hard to tell. Since this section is the valuable novel contribution of this paper, I strongly encourage to rework it substantially for terseness and clarity.

Here are just a few comments on the initial parts of section 2, (comments similar in spirit likely apply to the latter part):

- The section starting at line 127 ("Second, ...") seems to more appropriately be placed with the discussion of interacting biradicals later in the manuscript.

- There is a notational inconsistency between omega_0 (dipolar frequency in biradical with B-spin number 0) and \tilde\omega_l (dipolar frequency in biradical with B-spin number l) - why tilde in one case and not the other?

- The approximation leading to eq.(10) is handy, but its range of validity is not stated. \omega_n\tau_1 must be smaller than about 0.5 for it to be reasonable. This should be

mentioned. Does this have any consequence in the context of the experimental data?

- The terms "filtering" and "pre-filtering" are used in several places, including the title. I have to admit that I do not completely understand what this term is meant to indicate, so I am not able to judge whether the associated statements are valid. What is the definition of filtering? Can this be clarified?

- The discussion between eqs. (12) to (15) is confusing. It seems to start out with an ensemble average, but then some new notation is introduced, such \tilde{B}_S and B_t(\tau), without defining equations. What does the tilde indicate? What does the S subscript indicate (and the lower-case subscript s that appears elsewhere several times)? And what does t subscript in B_t represent? It's all a bit unpenetrable. Also, to what degree is eq.(15) going beyond just an ensemble average of the detected signal using the density from eq.(12)?

- Eqs.(9) etc. using the symbol V with incrementing subscripts to indicate density operators at various points in the sequence. Since the earliest Hahn papers, or even Bloch, V is universally used to indicate the signal intensity, i.e. something proportional to the trace of density times a detection operator). Why not use the standard notation \sigma for the density operator, as was done in section 2.1? Also, why not use the actual time points instead of the subscripts, like was done in Eqs.(2)-(6).

- Eq.(17) is said to have "parabolic shape curved down" - as a function of what? It seems like it must be seen as a function of time t, where tau1 = tau1_0 + t and tau2 = tau2_0 - t. The scanned time t should be defined, probably together with the SIFTER sequence in Fig.1. Then, one can write tau1(t)*tau2(t) in Eq.(17), and this is then obviously parabolic in t.

[3]
Equation (40) seems to be the central result. Is it possible to add a figure that plots the various components of the SIFTER signal (and the SIDRE signal) and thereby assists in visualizing the anatomy of the signal?

[4]
The experimental figures 2 and 4 show the divisions of the SIFTER and SIDRE signals. While Eq.(40) decsribes the SIFTER signal, what is the expression for the SIDRE signal? Is it \tilde{B}(tau1,tau2)? It would probably be helpful to introduce a notation such as V_SIDRE(tau1,tau2) = ... for clarity.

[5]
The "SIDRE" signal is basically the 1D antidiagonal of the 2D signal of the refocused two-pulse echo, V(tau1,tau2). 2020 Bahrenberg et al show several plots of V(tau1,tau2), both experimentally and theoretically. It might be good to refer to this work a bit more explicitly in the context of the discussion of the SIDRE sequence and the SIDRE experimental data.