

Magn. Reson. Discuss., community comment CC1
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Reply on RC1

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Community 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-CC1>, 2022

Dear Frédéric, many thanks for a number of useful suggestions and for the overall positive judgement on our manuscript. While we are discussing within the authors the detailed step-by-step response and corrections, I would like to ask for some additional clarifications regarding the following three points in your reviewer report.

Your comment for L159: w_l and w_m are confusing. My understanding is that there is some redundancy here though I do not think it matters. w_l refers to the intramolecular dipolar coupling of the biradical l but not the spins themselves, while l_m is for the coupling between two spins l and m belonging to two different molecules. I would use upper case W_m for intramolecular, and lower case w_m for intermolecular. This would ease understanding where intermolecular couplings contribute.

My question: The frequency w_l is written with one index (this is the spin index, not the molecule index) because there are only $N/2$ different intramolecular frequencies. Summing over all spins (only single index summation is needed here) would just count all these frequencies exactly twice, which is convenient enough to handle. The intermolecular frequencies need to be summed in some cases over two indices, and there are $N(N-2)/2$ different w_m frequencies, i.e. here two indices are really necessary. Thus, I would actually advocate that we stay here with the originally set abbreviations, unless you strongly insist. How do you see this?

Your comment for Eq 9: Since you use the same approach as in 2.1, I would suggest, for consistency, to use $\sigma(2\tau_1 - \Delta t)$ should be used not V .

My question: I would personally prefer to keep σ in the section 2.1 and V in the section 2.2 and later to discriminate between the two-spin density matrix and the multi-spin density matrix. It is however true that we omitted indicating the time points for the V . I would suggest writing $V(2\tau_1 - \Delta t) = V_1 =$ equation, and so on for all the equations with V . Would this be acceptable for you?

Your comment for the L170: $\tan(\omega\tau_1) \cdot \cos(\omega\tau_1) \approx \omega\tau_1 \cdot \cos(\omega\tau_1)$ is a disturbing approximation. It is far worse than a simple Taylor expansion of \sin . I understand why you do this to have a product over all N , I would do it first, then apply the approximation of $\tan(x)$ as $\sim x$. Actually you explain this later, L258 "In equation (21) we can add the missing factor \cos "

My question: Here, I am not sure I understand the comment. The relation $\sin(x) = \tan(x) \cdot \cos(x)$ is exact, ($x = \omega n \tau 1$). In the next step we just write the first Taylor term for the $\tan(x)$ while keeping the whole $\cos(x)$ function unchanged. This is correct up to the linear terms on x , but keeps some terms $\sim x^3$, which is not important within our approximation level. In fact, in the final equation for V we get the most significant term $\sim x^2$, and the next order term, which we partially neglect and partially keep in the $\cos(x)$, would be $\sim x^4$. Could you, perhaps, explain in a bit more detail where you see a problem in our approximations, and what is the suggested change?