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Magn. Reson. Discuss., community comment CC1
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# Comment on mr-2022-9

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Community comment on "Visualization of dynamics in coupled multi-spin systems" by Jingyan Xu et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-9-CC1, 2022

Dear Jingyan, Dmitry and Danila

Thanks for advancing MR field!

I read your preprint and have a few comments and questions regarding your work.

in the intro you write, “Most NMR textbooks visualize the motion of a single spin-1/2 (or an ensemble of spins) using the Bloch vector.”

*I understand this because it gives us a simple rule to explain and describe spin evolution. Moreover, there are modified rules for the week coupling case that use product operator formalism. How do we know what they are useful? Because they give us an excellent tool to predict an effect on paper before measuring it.*

In conclusion, you write: “AMP/AMC surfaces conveniently represent symmetries of density matrices and allow spotting their presence (orientation, alignment, etc.) or absence even when direct analysis of density matrices is not obvious. <..> The presented AMP/AMC surface approach allows visualizing complex dynamics in multispin systems and may find applications for describing hyperpolarization experiments”

*I miss new insights into spin evolution. I do not understand how this approach can help to explain spin evolution simpler or predict something new.*

Some other comments:

*Comment 1. I can guess Figure 1c, need corrections. Something like Fk,mF->Fk,mj, Fl,mF->Fl,mi, for mi,mj<Fl, rhoFlFk_mF,mF->rhoFlFk_mi,mj and then in the caption only mF=mi=mj were used for visualization.*

*Comment 2. L 135* “Lastly, Fig. 5E, which measures the out-of-phase coherence reveals extra information not covered by Fig. 5B, i.e., the singlet-triplet coherence, ˆI1y

ˆI2x−ˆI1x ˆ 135 I2y, is transiently formed during the experiment."

*- It was your free choice not to plot o-o-p coherence on B, which you can add, and then again no new information I can gain from the visualization. Or I'm I missing something?*

*Comment 3. Fig 6. T1 and T2 are the unfortunate choices because they have some specific mining in NMR. Maybe small tau instead?*

*Comment 4. Line 150*: "Dynamics of the AMC surfaces shown in Fig 6D-F is more intricate. Their motion is a superimposed oscillation of shapes with a period of T2 = 1/J and a slow precession about the x-axis with the above-mentioned period of T1. From the visualization, one may conclude that in-phase and out-of-phase zero quantum coherences give rise to the doublet shown in Fig 6B"

*- What is your observable? If something evolves with the same frequency it does not mean that it is the reason for the signal (i'm not saying that it is the case here).*

*- You need to explain how the evolution of ZQC results in the observation of the ULF spectrum.*

*Comment 5 :* "Code availability. The software code for the graphics shown in this paper is available from the authors upon request"

*I hope this statement will be not acceptable for any journals and MR will have a strict policy on publishing all scripts together with the paper or EU-repositories with doi like zenodo.org*

*With kind regards*

*Andrey Pravdivtsev*

Please also note the supplement to this comment:
https://mr.copernicus.org/preprints/mr-2022-9/mr-2022-9-CC1-supplement.pdf