

Magn. Reson. Discuss., community comment CC2
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Reply on CC1

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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-CC2>, 2022

Andrey, thank you for valuable comments. The most important message we want to emphasize is that all information about the spin system is contained in the density matrix (DM), thus, no "new insights into spin evolution" are necessarily expected from AMP/AMCs. However, such visualization approach allows seeing DM symmetries in a more convenient way - thus, new insights may potentially be generated by an inspired reader. Imagine a state ($I1zI2z$) globally rotated by 33 degrees about x-axis. Good luck understanding what state it is by looking at DM directly (not that it is impossible): all elements will be populated when DM is written in the original basis. Simple visualization algorithm presented in this work produces the surface from which the symmetry (alignment) is immediately obvious. In addition, Appendix C shows that DM and the visualized surfaces form one-to-one map. We plan to elaborate on this subject more in a revised version of the manuscript and shift the focus from "new insights" into convenience of observing symmetries.

Comment 1: We plan to modify Figure 1 in the revised manuscript to enhance explanation and reduce confusion.

Comment 2: See above comment about information content in the visualizations. In order to keep one-to-one correspondence between the DM and the visualized AMP/AMC surfaces, we present the out-of-phase coherence for completeness.

Comment 3: We modify the labeling in the revised version.

Comment 4: Very good comments, for the AMP/AMC surfaces – it is probability that is important, not necessarily the measured property. However, in a particular case of in-phase zero-quantum coherence ($I1z-I2z$) represented by AMC surface in Figure 6D-E, the intersection of this surface with positive z-axis represents directly a measured signal in ZULF NMR experiments. We will elaborate on this subject in more detail in the revised manuscript.

Comment 5: The code will be provided although we followed several published examples in the MR journal where such statements about the code availability were provided.