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Reply on RC3

Jingyan Xu et al.

Author 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-AC4, 2022

Dear Malcolm, we thank you for the critique. The paper was substantially rewritten and now the visualization approach is based on the use of generalized measurement-related operators. We note that this approach provide us with valuable information which is not easy to grasp through direct observation of numerical values of the density-matrix elements. First, the action of global rotations applied to the density operator is directly reflected by the rotations of the plotted surfaces (see new Fig. 3). Second, there is a close relationship between the density matrix coherences and the symmetries of the plotted surfaces (see new Fig. 4). Third, our visualization allows one to quantitively understand the measured ZULF NMR spectrum by looking at the intersection of the surface with an axis representing sensitive direction of a magnetometer. As an example, the ZULF NMR spectrum of an AX system is now pictorially explained through our visualization. Specifically, we explained the small asymmetry of the doublet centered at J-frequency which is not easy to grasp through the product operator formalism.

We also improved the text by simplifying some mathematical notations and by using terminology which is more familiar to the NMR community. In simple words, our visualization is now performed by plotting measurements with zero-quantum Hermitian operators rotated along various directions.

Despite coherences (visualized via AMC surafes) were indeed off-diagonal elements of the density operator written in the total angular momentum basis (i.e., Hamiltonian eigenbasis at zero magnetic field), we agree that excessive use of the “coherence” terminology did not add additional value to the paper. For this reason, we abandoned the term "AMC surfaces" in the updated version of the paper and now refer to the visualized surfaces directly via the measurement operators.

Regarding the software availability. The statement “The software code for the graphics shown in this paper is available from the authors on reasonable request” was a direct copy (except deletion of the word reasonable) from the following article published in Magnetic Resonance (see https://mr.copernicus.org/articles/2/395/2021/). Nonetheless, we gladly provide the code in the revised version of the manuscript.

Taken together, thanks to your comments, we believe the paper is significantly improved an, hopefully, it is now more accessible for the magnetic resonance community.