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Comment on mr-2022-9

Malcolm Levitt (Referee)

Referee 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-RC2, 2022

The paper describes a visualization tool for the representation of density operators in multiple-spin systems. The approach is inspired by the DROPS software of Glaser and co-workers, and shares with that work most strengths and weaknesses. The strength is a graphical representation which might possibly lead to a helpful visualization of complex spin dynamics, sidestepping the need for complex mathematics, and possibly help inspire new procedures or give new insights. The main weakness is that although the tool allows a pretty graphical representation of the mathematics, it does not replace the mathematics, at least not as far as I can see. So the result seems to be pretty graphics (which I am all for) but not with evident real utility, in contrast to the Bloch vector picture, from which many NMR effects and experiments have been derived.

So I am not yet convinced of the utility of this representation. Furthermore I cannot see exactly how it works, and the authors do not help since they choose a mathematically dense exposition which is very hard to follow, right from the beginning. Despite my best efforts I cannot understand equation 1 and the following equations. It may be that the terms used by the authors are self-evident to the atomic physics community but I suspect that most readers of this journal will, like myself, struggle greatly with it. For this to work the authors must make far greater efforts to express themselves in language comprehensible to us mere magnetic resonance mortals. What on earth is the "block (Fk, Fk)"? Scientists on the same level of mathematical physics as myself will need to be led far more slowly through this material, using helpful simple examples on the way.

In addition the authors introduce the term "angular momentum coherence (AMC)". I suspect that the term coherence is used here to mean something very different from its standard usage in magnetic resonance, as defined by Ernst and co-workers (an off-diagonal density operator term, when written in the Hamiltonian eigenbasis). I am not sure though since I cannot follow the authors' meaning. In general I do not think a redefinition or loose usage of this fundamental term is advisable.

In summary I am sympathetic to the aims of this paper but find the presentation

impossible to follow. In addition, I am far from convinced of its usefulness, but recognise that it could be of value if explained well enough and made sufficiently accessible.

On the issue of accessibility, I agree with another referee that it is not longer acceptable, for work of this kind, to say that the code is available on request.