

Magn. Reson. Discuss., referee comment RC3
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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-RC3>, 2022

A further comment: The article emphasizes the total spin angular momentum quantum number (denoted F , I believe). Off-diagonal density operator elements spanning states with different values of F appear to be called "angular momentum coherences" (AMCs). This nomenclature and analysis might be appropriate for atomic physics, where the Hamiltonian has isotropic, or near-isotropic symmetry. However this situation is rarely encountered in magnetic resonance of bulk matter, since we hardly ever deal with isotropic systems. Trivially, the application of a strong magnetic field breaks isotropic symmetry (leading, amongst other things, to the Zeeman effect, upon which most magnetic resonance is based). Even the solution NMR of isotropic liquids does not involve an isotropic Hamiltonian. Very often, chemical shift differences and other interactions break the symmetry further. In most cases these are not small perturbations but completely break the isotropy of the spin Hamiltonian. There are rare exceptions, such as zero-field NMR.

Since high-field NMR almost always uses Hamiltonian eigenstates that do not have well-defined values of F , I do wonder what utility this diagrammatic approach might have. Furthermore, although the concept of AMC's "angular momentum coherences" might possibly mean something in atomic physics, I suspect that it has no, or little, relevance to the vast majority of magnetic resonance experiments, and probably conflicts with the conventional use of the term coherence in magnetic resonance - namely a coherent superposition of Hamiltonian eigenstates.

I think the article will not be appropriate for the magnetic resonance community unless these sharp differences between the atomic spectroscopy and bulk magnetic resonance contexts are highlighted more clearly.