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Comment on mr-2022-9

Geoffrey Bodenhausen (Editor)

Editor 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-EC1, 2022

This paper introduces a graphical convention for the representation of various forms of spin order in coupled systems.

Personally, I find figures such as Fig. 4B perfectly adequate, and I fail to see any advantages in ‘AMC’ pictures such as those in Fig. 4E and 4F. True, the ‘AMP’ pictures of Fig. 4 C and 4D are even less informative. Likewise, in Fig. 5B it would have been easy to add a line to show the time-dependence of the singlet-triplet coherence. I would prefer to call it a long-lived coherence or LLC.

The problem with many graphical representations is that, while their beauty and elegance may be obvious to their inventors, they may remain opaque for many readers.

The beauty of some non-trivial trajectories on Bloch’s sphere is one of the very few exceptions that confirm the rule. Their success is mostly due to the unmatched talents of the regretted Ray Freeman and some of his students like Gareth Morris who illustrated DANTE’s spiraling descent to hell, and Malcolm Levitt’s composite pulses.

I myself have made several ill-fated attempts to become famous by introducing various graphical conventions. Thus I failed to convince Ray that phase corrections in 2D spectra should be represented on the surface of a taurus rather than on a sphere (Ray, who would never make any disparaging comments, kindly referred to ’Geoffrey’s doughnuts’.) A few years later, I tried to represent a double-quantum coherence in deuterium NMR by a ‘d’ orbital with two positive and two negative lobes in the equatorial plane. Bob and Gitte Vold, with whom I was working in those days, wisely discouraged me. On the occasion of Xmas 1978, I offered them some ‘double-quantum cookies’ by adapting the shape of a Swiss cake mold. Those cookies were not intended to gain celebrity status.

While at ETH with Richard Ernst, we invested a fair amount of time in graphically representing transformations of product operators by so-called ‘windmills’ that show triads of non-commuting operators. Nobody ever uses these. Likewise, we chose to represent coherences by squiggly lines drawn onto energy level diagrams, using dashed lines for imaginary terms, and solid lines for real operators. Again, nobody ever cared about these carefully designed pictures. On the other hand, our representations of populations of eigenstates in terms of positive and negative deviations from the demagnetized state were often misunderstood and frequently misused. We affectionately referred to our black-and-white ‘ping-pong balls’, but Richard disapprovingly called them ‘Boppeli’, using a disparaging Swiss-German diminutive that did not bode well. How right he was.

The only graphical convention from this period that had some sort of success (cited 1420 times in Google's beauty contest) appears to be our 'coherence transfer pathways'. The graphical conventions that show the path through different levels of zero-, single- and p-quantum coherences are commonly used to clarify what such-and-such a pulse sequence is supposed to achieve. However, it seems that these pictures are rarely used to derived phase cycles, and few appear to appreciate the implications of selecting 'mirror' pathways to obtain pure phase signals.

With Norbert Müller, we developed an elaborate graphical convention (no doubt too elaborate!) that keeps track separately of the coherence orders 'p' and tensor ranks 'l' for three methyl protons M and a neighboring proton A in AM3 systems. Figure 7 in 'Cross-Correlation of Chemical Shift Anisotropy and Dipolar Interactions in Methyl Protons Investigated by Selective Nuclear Magnetic Resonance Spectroscopy' by N. Müller and G. Bodenhausen, J. Chem. Phys. 98, 6062-6069 (1993), may serve as a warning for future generations against over-sophistication. I intend to upload this figure on 'MR discussions' in a separate pdf file for the amusement of today's readers. If one can trust Google, the paper was cited a whopping 16 times in 29 years.

With Urs Eggenberger, we tried to develop a graphical scheme that allows one to sketch transformations of product operators under shifts and couplings without the need to write out bulky trigonometric expressions in "Modern NMR Pulse Experiments: A Graphical Description of the Evolution of Spin Systems" by U. Eggenberger and G. Bodenhausen, Angew. Chem. Int. Ed. Engl. 29, 374-383 (1990). The objective of this hapless paper is actually more ambitious than the aim of the paper submitted by Budker et al. Yet, despite our best efforts, and despite the reputation of Angewandte Chemie, our paper was a complete flop, since it was only cited 24 times in 32 years. (I firmly reject the widespread idea that high citation numbers correlate with originality, but concede that low numbers indicate poor impact.)

Yet, to our surprise, our 'coherence transfer pathways' turned out to be most successful in solid-state NMR, in particular for quadrupolar nuclei. Phil Grandinetti invented so-called 'transition pathways', which show successive transformations of single-transition operators representing coherences, or of polarization operators representing populations (J. Am. Chem. Soc.,130, 10858–10859, 2008.) This idea evolved into a paper entitled 'Symmetry pathways in solid-state NMR', by P. J. Grandinetti, J. T. Ash, and N. M. Trease, Progress in Nuclear Magnetic Resonance Spectroscopy, 59, 121-196, 2011. According to Google Scholar, it was cited 47 times in 11 years, hardly a resounding success.

So I do not expect the paper submitted by Budker and co-workers to become a 'citation classic'. Fortunately, 'Magnetic Resonance' is not striving to optimize its impact factor. We cannot exclude that some younger scientists may find inspiration in their graphs. It would therefore be counter-productive to reject this paper.

As pointed out be one of the reviewers, it is not acceptable to write 'The software code for the graphics shown in this paper is available from the authors upon request.' It should be down-loadable form a server.

As editor of Magnetic Resonance, I strongly object to the authors' use of the word 'coherence' in their abbreviation 'angular momentum coherence (AMC)'. Whatever witty name they may choose for their graphs, our scientific community should not allow them to get away with such a misleading abbreviation that can only create confusion. Perhaps 'Local angular momentum probability (LAMP)' would convey the authors' ideas? Some readers might find this abbreviation enlightening.