

Magn. Reson. Discuss., community comment CC3
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Review of mr-2022-18

Bernhard Bluemich

Community comment on "Simulation of NMR spectra at zero and ultralow fields from A to Z – a tribute to Prof. Konstantin L'vovich Ivanov" by Quentin Stern and Kirill Sheberstov, Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2022-18-CC3>, 2022

General comment:

I really enjoyed reading this paper. It reminded me of my time as a PhD student, when I tried to understand the density matrix formalism and program the transverse magnetization response to some odd excitation using assembler code. In those days long gone I found the then recent paper by P.D. Buckley, K.W. Jolley, D.N. Pinder "Application of density matrix theory to NMR line-shape calculations", PNMRS 10 (1975) 1-26 most helpful as it gave hands-on examples which I could adapt to my own case of interest. Compared to that old paper, the manuscript at stake is written even more in a tutorial style, working out the details of the A_3X system as an example. In my view this is a valuable guide to beginning PhD students interested in ZULF NMR. Clearly this manuscript is not a review, nor does it cover all common cases encountered with ZULF NMR, but I find it to be quite useful as a starting point for one's own simulations. I recommend it to be published following revision. In particular, the corrections and comments voiced in the discussion so far should be considered and implemented so long as the length of the manuscript can largely be maintained.

Detailed additional comments:

Line 20 ff: "Increasing magnetic field strength boosts the sensitivity thanks to higher Boltzmann nuclear polarization and higher Larmor frequency". Although stated many times in the literature, this only applies to high-resolution spectroscopy at constant linewidth in frequency units. It is the peak amplitude and not the peak integral in the spectrum that defines the sensitivity. (This raises the question of the "homogeneity" of the zero-field and its impact on spectral resolution and sensitivity at a given polarization.) Perhaps one can write "increasing the field strength while maintaining the linewidth ...".

Line 133: Figure 1B

Line 170: What defines the directions of the axes at zero field?

Lines 224 and 226: Are "density operator" and "density matrix" used synonymously? That is confusing to the beginner.

Equation (19) and throughout the entire manuscript: The format of constants, variables, functions is inconsistent. This poses extra barriers for a student struggling to understand the math. The formatting rules apply independently to the quantity under consideration and its superscripts and subscripts. For example, the subscript "eq" in (19) is not a variable and should not be written italic.

Lines 335: What is a "Fourier transform function"? The Fourier transformation is an operation, the result of which is a transform. Both, input and output of the Fourier transformation are functions. See also line 345.

Lines 399, 416 "... multiply the frequency domain signal" Should probably read "... multiply the abscissa of the frequency-domain signal ...".

Line 435, "Hermitian": Charles Hermite was a French mathematician. Consequently, the attribute referring to his name is correctly spelled "Hermitean". Admittedly, contrary to the older literature, one often finds "Hermitian" in the modern literature. You may want to pay tribute to the correct spelling of his name in the manuscript.

Caption to Fig. 5 and elsewhere in the text: "with a zero-filling of 65'536 points" should be replaced by "with zero filling to 65,536 points", because you did not fill in 65,536 zeroes.

Overall the manuscript is well written, with just a few language issues, which I am sure, the Copernicus editors will pick up.