

Magn. Reson. Discuss., referee comment RC5
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Comment on mr-2022-18

Anonymous Referee #4

Referee 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-RC5>, 2022

The work from Q. Stern and K. Sheberstov is a tutorial paper addressed to PhD students approaching NMR experiments simulations at ultra-low or zero field.

Despite the manuscript is well written and over all correct, I struggle to see a real pedagogical aim in this work. In my honest opinion, I doubt that first year PhD students will be able to open their MATLAB and start to run NMR simulation thanks to this manuscript. I must agree with Reviewer 1 about the fact that the authors assume a lot more of the readers' pre-knowledge than what they think. Through the text, apart some NMR theory that can be found in any topic specific textbook (e.g. Spin Dynamics from Prof Levitt), I could not see any real trick that would "carry by hand" the newbie from analytical formulas to computation. Moreover, especially at the beginning, jumping straight to ZULF simulation might be confusing for the non-experts. The paper could be useful for a broader audience if a "standard/high-field" NMR section was added.

The following is just a suggestion, but, why not starting with a very simple system (non-interacting spins $\frac{1}{2}$ at thermal equilibrium with Zeeman interaction only, no propagation of the density matrix yet just CW style) and show step-by-step how to go from the Hamiltonian to the spectrum in MATLAB, reporting even chunks of code into the main text. Then, we can add the J-coupling and see how the spectrum changes, propagate the density matrix etc.

As a first year PhD student I would love to find in the literature something like this!

Below some minor details:

Line 27: the second "interaction" is redundant

Line 41: add a reference after "coils" about OPM detection for ZULF

Line 42: I would remove "This simple idealization of"

Line 427: "positioned" instead of "position"