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Magn. Reson. Discuss., community comment CC6
https://doi.org/10.5194/mr-2021-65-CC6, 2022

Comment on mr-2021-65

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Community comment on "Radiation damping strongly perturbs remote resonances in the presence of homonuclear mixing" by Philippe Pelupessy, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-65-CC6, 2022

This paper is yet another wonderful demonstration of the one-to-one relationship between quantum mechanical spin simulations and experiment. I commend the authors on both the measurements and calculations that are more than supportive of the claims. That said, I am not at all surprised by these results. Years ago I considered similar effects in simulations – effects of a radiation damped resonance with an uncoupled smaller resonance nearby (a so called coupled pendulum) and with a coupled smaller resonance nearby – to explore new spin physics and non-linearity. (Indeed, I recommend the author digs into the appendix in Sleator and Hahn's PRB vol. 36, pg. 1969, yr. 1987 spin noise paper. The magnet, probe and sample coupling the author has access to may be enough to cause the frequency pulling of nearby resonances and lead to some new ideas) I never played around with the more useful and sophisticated pulse sequences studied in the manuscript and I am glad the author chose to write this up. I have no serious issues with the manuscript as is just some questions that the author might consider mentioning to make the paper more accessible to folks other than myself, Tom Barbara and Malcom.

In short, when does the normal NMR public need to worry about these effects eg. what concentrations of protonated water or solvent are tolerable ?

It is clear from the manuscript that the sample, 100 M proton with solute, and the spectrometers, an 800 and 600, were chosen to make the effect pronounced. The author mentioned at the end of the theory and discussion section that the effect was more pronounced on the system using a cryoprobe. It is also mentioned at the end of the conclusion that the effect can be removed by saturating or dephasing the radiation damping causing spins. I think the greater NMR community would benefit by an empirical estimate of the maximum proton concentration tolerated by the conventional pulse sequences before the predicted radiation damping effects corrupt the results. Yes, 100 M protons on a 600 with a cryoprobe and 100 M protons on an 800 with a normal probe, display these effects. Does one always have to use 100 % D2O to avoid the RD effect ? I think it boils down to simple probe Q and how much water is present – or you could just calculate the RD time constant that depends on both Q and the magnetization and assign a cutoff value. Such a brief comment could be tacked on the end of the conclusion if the author agrees.