

Magn. Reson. Discuss., referee comment RC1
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Comment on mr-2021-43

Malcolm Levitt (Referee)

Referee comment on "Effects of radial radio-frequency field inhomogeneity on MAS solid-state NMR experiments" by Kathrin Aebischer et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-43-RC1>, 2021

This is a very fine paper describing highly detailed state-of-the-art theory and simulations of "radial radio-frequency inhomogeneity" effects in MAS NMR. The most unusual aspect of this type of inhomogeneity is that since the phase of the applied rf field varies in space, and a volume element of a rotating sample traverses the inhomogeneous field, the rf field experience by the nuclear spins acquires a periodically time-varying phase, which can interfere with the performance of NMR experiments. The authors analyze these effects closely for a variety of sample rotors and pulse sequences, and conclude that the effects are usually too small to have serious consequences.

In this conclusion they may well be right. However they may have missed at least one prior report in the literature. In 1988 (doi.org/10.1002/ijch.198800039) rotary resonance recoupling experiments were reported in which an unanticipated peak appeared in the centre of the expected dipolar doublet (see Fig.4a in that paper). The following discussion, around equation 27, postulates a spinning-induced periodic phase modulation of the radio frequency field, due to inhomogeneity in the field direction, of the same type analysed in the current paper (this was actually 3 years before the Goldman article cited by the authors as the seminal reference). Simulations including a highly simplified model of this phase modulation did reproduce the central peak (figure 6). It would be interesting to know whether the far more sophisticated calculations performed by the authors verify — or disprove — this finding.

Apart from this comment which might require some minor changes to the paper the only criticism I have for this excellent piece of work is that the use of radians as the phase unit makes some of the figures needlessly hard to interpret. I suggest they plot the phase in units of degrees for ease of interpretation — or if they really do not like degrees, plot phase divided by π , or similar.