

Magn. Reson. Discuss., community comment CC2
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Comment on mr-2022-8

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Community comment on "The effect of spin polarization on double electron–electron resonance (DEER) spectroscopy" by Sarah R. Sweger et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2022-8-CC2>, 2022

The paper is important contribution in the field of dipole spectroscopy, it provides rather clear picture of the spin dynamics effects.

I think it would be suitable to cite our early theoretical paper (attached) Maryasov A.G., Dzuba S.A., Salikhov K.M. Spin polarization effects on the phase relaxation induced by dipole-dipole interactions. J. Magn. Reson. 50: 432-450, 1982. There we demonstrated that out-of-phase component will appear in the case of finite value of $\chi(B,T)$ given in Eq.(5) of the manuscript, see Eq(29) of the old paper. We studied dipole line broadening that time, and spectral diffusion caused by d-d interaction in 3D system with randomly distributed PCs, so didn't concentrate on out-of-phase signal. Now those results may be treated as background signal calculations. High Boltzmann polarization of spins in pair of radicals leads to the triplet character of the pair initial state regardless of the strenght of dipole spin coupling, equilibrium density matrix is proportional to $S_{1z}+S_{2z}+cS_{1z}S_{2z}$, where c is a non-zero constant even when d-d interaction is negligible. High Boltzmann polarization also reduces spectral diffusion effects in weakly coupled systems. It seems to me that our old paper is relevant to be cited.

Please also note the supplement to this comment:

<https://mr.copernicus.org/preprints/mr-2022-8/mr-2022-8-CC2-supplement.pdf>