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Magn. Reson. Discuss., author comment AC1
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Reply on CC2

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Author 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-AC1, 2022

Dear Tom Barbara (in answer to the two comments),

Thank you for your comments and for pointing out the references (which give analytical solutions to the modified Bloch equations in presence of an RF field for the case that the RD field is exactly perpendicular to the transverse magnetization). I am finishing a revised version which addresses the reviewers' and your comments in detail. It is an interesting question whether there is a connection between the "imaginary resonance offset" and the effect observed in this article. Another relevant reference in this context may be Warren, Hammes and Bates, J. Chem. Phys. 91, 5895-5904 (1989), which analyzes the behavior of the solvent spins under a continuous wave spin-lock. The net effect of the DIPSI-2 cycle on the *passive* spins, shown in figures 3-5 of the manuscript, is that the magnetization of these spins precesses away from the much larger spin-lock field (it has the effect of a real offset, an effective Hamiltonian dominated by a term proportional to I_z). In contrast, the magnetization of the *solvent* (the source of RD) is much better (although not perfectly) controlled by de DIPSI-2 spin lock (as you also stated), i.e. it stays very close to the *z* -axis after each mixing cycle for the conditions in figure 5 while it stays close to the *x*-axis for the conditions in figure 6. The analysis can be much simplified when one considers an even stronger field (as reviewer 2 suggests) on-resonance with the solvent. When the initial solvent magnetization is along the *x*-axis, this magnetization stays continuously almost perfectly locked along this axis and (neglecting relaxation) the RD field is constant, with one component parallel to the magnetization equal to $R_R\sin(\psi)$ and one term perpendicular to it along the *y*-axis equal to $R_R\cos(\psi)$. The latter component is efficiently (in analogy to the offset term) averaged out from the effective Hamiltonian by the DIPSI-2 sequence, while the first component is unaffected since it commutes with the RF field at all times. Note that ψ must not be zero in order for this effect to be present under these conditions (as reviewer 1 and Malcolm Levitt suggest me to discuss). Hence, the effect of the RD field on the dilute spins (after each completed DIPSI-2 cycle) is expected to be a nutation around the *x*-axis with a frequency of $R_R\sin(\psi)/2\pi$. Simulations (the actual DIPSI-2 sequence has always been considered) with an RF amplitude of 100 kHz confirm this. When the initial solvent magnetization is perpendicular (either along the *z*- or the *y* -axis) to the spin-lock field, the situation is different since the RD field becomes time-dependent. The net effect seems to be a nutation around the axis of the initial solvent magnetization with a frequency of about one half compared to the previous one. When the initial magnetization of the solvent is oriented arbitrarily, the situation is much more complex. Contrary to (my) intuition, the evolution of the solvent magnetization can be *strongly* influenced by the much weaker RD field when the initial magnetization is not

close to an orientation parallel to one of the three main axes.

Kind regards,

Philippe