

Dear Professor Levitt,

We are very thankful for your suggestions regarding the manuscript and your overall positive evaluation of the work. We fully agree with them and have made the following changes in the revised version:

1) Around lines ~75 the authors seem to claim a key original observation that the spin dynamics is restricted to the zero-quantum subspace. However, this observation is not entirely original - it appears in some relevant previous papers, for example <https://doi.org/10.1039/D2CP00899H> and <https://doi.org/10.1126/sciadv.abl3708> as well as the 2025 Mamone et al. paper which is already cited in the revised manuscript. It would be best to tone down the claim of originality here and include more references.

We fully agree that in a variety of previous works it has been shown that the zero-quantum subspace is highly relevant for the description of SABRE. In the proposed very nice works (10.1039/D2CP00899H, 10.1126/sciadv.abl3708), zero-quantum Hamiltonians have been considered, and therefore we clarified that these results primarily addressed coherent spin dynamics. We have modified the wording and adjusted the tone accordingly (lines 75–85):

Theoretical and computational studies of SABRE spin dynamics have attracted significant attention in recent years. In a number of works, it has been shown that the key contributions to polarization transfer in SABRE can be understood in terms of zero-quantum operators, highlighting the central role of the zero-quantum coherence (ZQC) subspace \citep{eriksson2022improving,snadin2024magnetic,markelov2021singlet,li2022sabre}...

In particular, Ref.~\citep{mamone2025coding} demonstrated that the description in terms of zero-quantum operators, including exchange and relaxation, successfully captures SABRE dynamics while reducing the dimensionality of the problem...

Here, we place these observations on a rigorous footing. We formally show (Fig.~\ref{fig1}B) that the Hamiltonian, relaxation, and chemical exchange superoperators in Liouville space possess a well-defined symmetry with respect to $\mathbf{\widehat{F}}$...

2) There are also some prior references on modelling the combined spin dynamics and chemical kinetics which should be cited and referred to, for example <https://doi.org/10.1002/chem.201901478>.

We fully agree that additional references would enhance readability. We have added four additional references related to modelling spin dynamics with exchange (10.1021/acs.jctc.1c00086, 10.1063/1.443791, 10.1002/nbm.2887, 10.1006/jmre.1999.1812) near line 45. Please note that the reference 10.1002/chem.201901478 has already been cited (line 285):

Although the full SABRE kinetics is generally non-linear (Pravdivtsev and Hovener, 2019), the linear approximation is adequate for most practical purposes.

3) In many places where the authors refer to "equivalence" it should be clearer that magnetic equivalence is implied, not chemical equivalence.

We fully agree that in some cases the term "equivalence" was unclear. Throughout the text, we have clarified that magnetic equivalence is assumed (e.g. lines 300, 305, 345, etc.).

We hope that the quality of the manuscript has been enhanced and that it now meets the high standards of Magnetic Resonance Discussions.

Sincerely,

Dr. Danil Markelov

On behalf of all authors