We thank the reviewer for their thorough and insightful feedback, which we greatly appreciate. Let us respond point by point.

1) The manuscript is carefully prepared and has no obvious errors. However, in its current detailed form, it is not always clear under which conditions the reduction of the Liouville space to a subspace is valid, and more importantly under which circumstances this approximation may break down. Clarifying these limits of applicability would strengthen the work.

We thank the reviewer for this remark. We agree that this point should indeed be clarified: the reduction is valid provided three conditions are met:

1. The Hamiltonian commutes with the z-projection of total spin, i.e., $[H, F_z] = 0$;
2. The initial density matrices of the free substrate (S) and the SABRE complex (C) commute with their respective F_z operators, i.e., $[\rho_C(0), F_{Cz}] = 0$ and $[\rho_S(0), F_{Sz}] = 0$;
3. The relaxation superoperator conserves the coherence order.

Strictly speaking, these conditions can be satisfied at arbitrary magnetic field strengths, for example at 10 T or at 1 μT. However, they are not met in the presence of transverse RF fields, in which case $[H, F_z] \neq 0$ and our assumptions no longer hold. Our approach is particularly valuable for ZULF rather than for high-field applications, because under ZULF conditions, where microtesla fields enable strong coupling between heteronuclei and protons, nontrivial "spontaneous" dynamics (i.e., without RF pulses) can occur. This point will be clarified in the revised version of the manuscript.

2) Furthermore, the manuscript appears to focus primarily on ZULF NMR, although the authors suggest that the proposed methodology could be applied more broadly. It would therefore be beneficial to elaborate on how this approach could be extended to high-field NMR experiments, where, for example, the equivalence of methyl and methylene groups might also be exploited.

We thank the reviewer for this thoughtful comment. As noted in our previous response, our approach is not suitable for high-field applications because conventional high-field NMR experiments typically rely on RF pulses to induce nontrivial spin dynamics, which violates the conditions under which our reduction is valid. For high-field NMR simulations of multi-spin systems, the well-established SPINACH package (Kuprov, I. (2018). Large-scale NMR simulations in liquid state: A tutorial. *Magnetic Resonance in Chemistry*, 56(6), 415–437) provides an excellent framework. In the revised version of the manuscript, we will clarify that our approach is specifically intended for low-field regimes.

3) In this context, the authors should also reference prior efforts aimed at simplifying spin dynamics calculations through permutation symmetry. Relevant examples include, but are not limited to, the work of I. Kuprov (https://doi.org/10.1016/j.jmr.2007.09.014) and S. I. Doronin (https://doi.org/10.1134/S1063776111130036).

We thank the reviewer for bringing these important references to our attention. These are excellent works related to the SPINACH package, and we will certainly cite them in the revised version of the manuscript.

4) Finally, a minor point - line 410 appears to be missing an important reference and should be corrected.

We thank the reviewer for pointing this out. Indeed, a relevant reference was inadvertently omitted, and this will be corrected in the revised version of the manuscript.