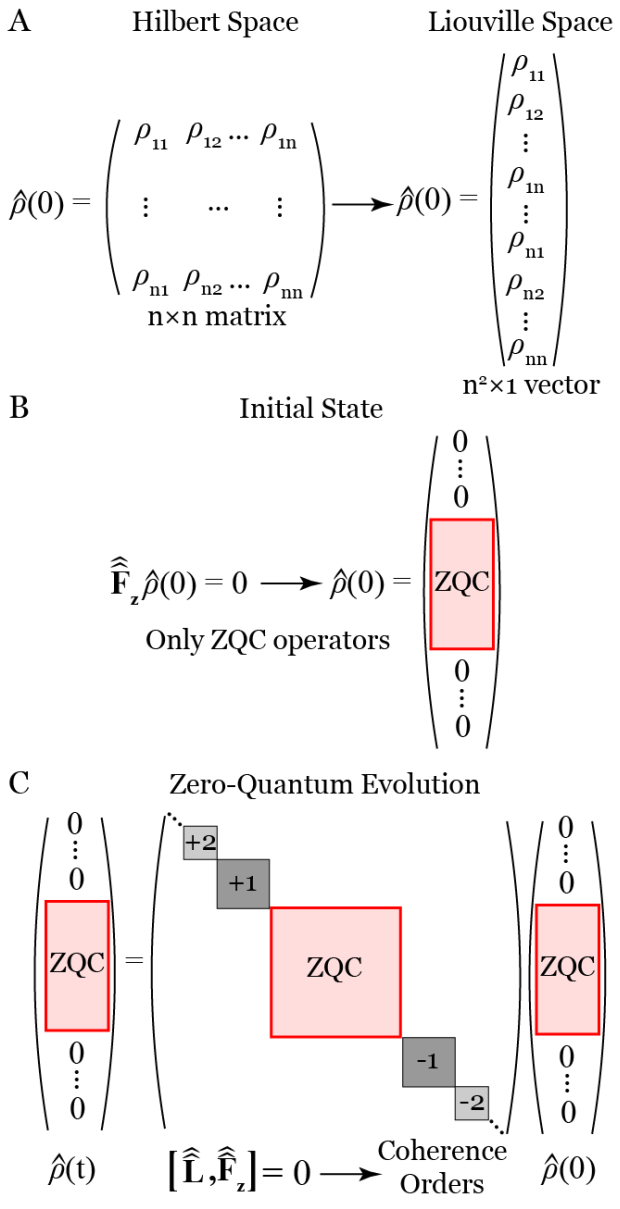
We sincerely thank the reviewer for their thorough and thoughtful engagement with our work. The reviewer has clearly delved deeply into the manuscript, and we greatly appreciate the insightful comments and constructive suggestions, which we find very valuable for improving the quality of our paper. Below, we provide a point-by-point response.

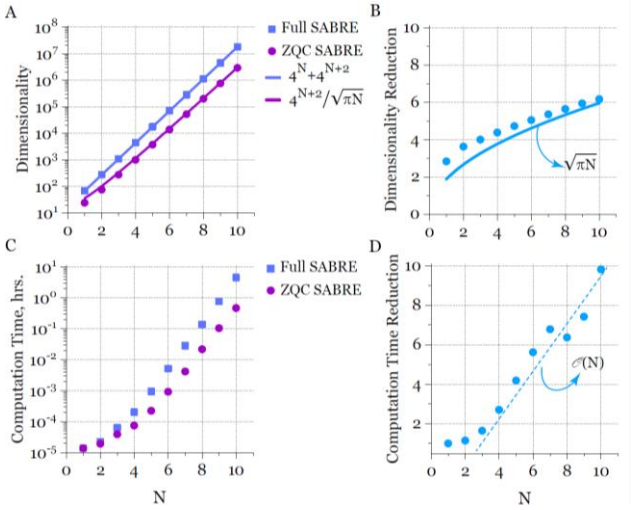
1) In particular, additional schematic figures illustrating the structure of the basis states, the relevant coherence pathways, and how the dynamics evolve within the reduced Liouville space would significantly broaden the readability of the manuscript. Figure 2 goes in this direction, but in its current form it remains too minimal to effectively guide the reader through the underlying physics.

We thank the reviewer for this valuable suggestion. We agree that a more detailed graphical illustration would significantly improve the accessibility of the material. In the revised version of the manuscript, Figure 2 will be replaced by the figure shown below. We believe this enhancement will help guide the reader through the underlying physics and improve the overall clarity of the manuscript.



2) Another aspect, admittedly not straightforward to quantify in general, that would strengthen the manuscript is a more explicit discussion of computational scaling. Providing, where possible, estimates of computational cost as a function of the number of spins and of the relaxation model would enhance the practical relevance of the work and allow a clearer assessment of the advantages over full Liouville-space simulations.

We thank the reviewer for this very useful remark. Inspired by this comment, we decided to add a subsection presenting a direct benchmark between the full and reduced approaches. As noted in line 340 of the original manuscript, the asymptotic reduction in matrix size scales with the number of spins as $\sqrt{N}$ when $\sqrt{N} \gg 1$. Furthermore, we now demonstrate that while the reduction in memory scales as $O(\sqrt{N})$, the computational cost scales as $O(N)$. A corresponding figure illustrating this scaling will be added to the revised version of the manuscript. We believe this addition will significantly enhance the practical relevance of our work and provide a clearer assessment of the advantages offered by our approach over full Liouville-space simulations.



As for the dependence on the relaxation model, we note that our approach is compatible with most relaxation models relevant to NMR, with the exception of CSA relaxation in the absence of axial symmetry (as noted in line 255 of the manuscript). Consequently, the choice of relaxation model does not substantially affect the qualitative conclusions regarding computational scaling or the validity of the reduction. For the purposes of our benchmark, we consider the random fluctuating fields model to be representative, as it captures the essential features of relaxation while maintaining compatibility with our symmetry-based framework.

3) Finally, it would be important to better position the present work within the existing literature. A closely related numerical framework has recently been presented at Euromar 2025 in Oulu (FI) and published (DOI: 10.1039/D5CP01773D), where Liouville-space reduction is achieved not only through symmetry considerations of the Hamiltonian and superoperators, but also by explicitly exploiting molecular symmetry and incorporating a dipolar (non–random field) relaxation model. In that case, the reduction emerges naturally from both the spin system topology and the underlying physical relaxation mechanisms, rather than from symmetry arguments alone.

We thank the reviewer for bringing this excellent and closely related work to our attention. Indeed, the authors propose a very similar approach also based on zero-quantum (ZQ) reduction, and we will certainly cite it in the revised manuscript. We also note that molecular symmetry is already incorporated in our simulations, as we treat methyl and methylene groups in terms of total spin, which directly reflects the underlying molecular symmetry. This point will be clarified in the main text to improve readability and better position our work within the existing literature.