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Singlet NMR Methodology in Two-Spin-1/2 Systems

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Giuseppe Pileio

*School of Chemistry, University of Southampton, SO17 1BJ, UK**The author dedicates this work to Prof. Malcolm H. Levitt on the occasion of his 60th birthday***Abstract**

This paper discusses methodology developed over the past 12 years in order to access and manipulate singlet order in systems comprising two coupled spin-1/2 nuclei in liquid-state nuclear magnetic resonance. Pulse sequences that are valid for different regimes are discussed, and fully analytical proofs are given using different spin dynamics techniques that include product operator methods, the single transition operator formalism, and average Hamiltonian theory. Methods used to filter singlet order from byproducts of pulse sequences are also listed and discussed analytically. The theoretical maximum amplitudes of the transformations achieved by these techniques are reported, together with the results of numerical simulations performed using custom-built simulation code.

Keywords: Singlet States, Singlet Order, Field-Cycling, Singlet-Locking, M2S, SLIC, Singlet Order filtration

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