

Optimal Control of Spin Dynamics

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Abstract: The field of optimal control theory offers powerful analytical and numerical tools to explore the ultimate performance limits of pulse sequences. In the last decade, these tools not only provided pulse sequences of unprecedented quality and capabilities, but also new analytical and geometrical insight and a deeper understanding of pulse optimization problems. Efficient numerical algorithms make it possible to develop robust time-optimal or relaxation-optimized pulse sequences, taking into account experimental limitations and imperfections, such as maximum pulse amplitudes, maximum pulse power, pulse inhomogeneity as well as transient effects associated with the switching of pulse amplitudes and phases.

Recent advances include time-optimal pulses for saturation and for maximizing contrast in magnetic resonance imaging (MRI), as well as robust broadband and band-selective pulses in nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy. The application of optimal control methods to the problem of hetero-nuclear decoupling yields not only significantly improved performance (1) but also unprecedented flexibility in the design of tailored decoupling sequences. In addition to individually optimized pulses, simultaneously optimized pulses provide significant performance gains by exploiting cooperative effects (2) and novel applications will be presented.

(1) F Schilling, LR. Warner, NI Gershenson, TE Skinner, M Sattler, SJ Glaser, Next-Generation Heteronuclear Decoupling for High-Field Biomolecular NMR Spectroscopy, *Angew. Chem. Int. Ed.* 53, 4475-4479 (2014).

(2) M Braun, SJ Glaser, Concurrently optimized cooperative pulses in robust quantum control: Application to broadband Ramsey-type pulse sequence elements, *New J. Phys.* 16 (2014) 115002.