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Design and Optimization of Solid State NMR Experiments for High Field Applications SETH MCNEILL, Electrical and Computer Engineering, JOANNA LONG, Biochemistry and Molecular Biology, University of Florida — Solid state NMR (SSNMR) has shown promise in examining biophysical problems such as the structure and dynamics of proteins in condensed phases. As magnet technology improves field strength, traditional analytical approaches for developing NMR pulse sequences, such as product operator formalism or average Hamiltonian theory, are no longer sufficient. In SSNMR, this is further confounded by the need to explicitly consider the spatial parts of the internal interactions for unoriented samples. Numerical methods for simulating the behavior of nuclear spins over a powder average have been developed. Concurrently, NMR spectrometers have converted from analog to digital RF technology making possible the development of more sophisticated pulse sequences. We have developed techniques to create optimized pulse sequences using RF fields of arbitrary phase and length leading to robust and attainable experimental parameters in high field conditions. Results for both simulating experimental data and developing more robust sequences for high fields are presented.

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