BCH5884 Final Project Proposal

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My research focuses on acquiring solid-state NMR (SSNMR) spectra of unreceptive nuclei, especially those with low NMR frequencies, low natural abundances, inconvenient relaxation characteristics, and most importantly, very broad patterns ranging from several kHz to tens of MHz in breadth (so-called ultra-wideline NMR (UWNMR) spectra). Previous work in the research group has established two widely-used methods for the acquisition of UWNMR spectra using direct excitation and broadband adiabatic cross-polarization (BRAIN-CP) techniques, which feature a special class of frequency-swept pulses known as wideband uniform-rate smooth-truncation (WURST) pulses. The overarching aims of my research are (i) to design new pulses, pulse sequences, and methodologies for the acquisition of high-quality UWNMR spectra of unreceptive nuclei, and (ii) to develop a clear understanding of the influence of different classes of pulses and pulse sequences on nuclear spin dynamics using quantum mechanical modeling methods.

An understanding of how the nuclear spins behave under the influence of different pulses and pulse sequences will be accomplished by tracking the nuclear spin density matrices (**DMs**) through numerical simulations and developing clear numerical/graphical methods for monitoring this behavior. Crucial to the understanding of evolution of spin polarization under the influence of pulses and NMR interactions is the development of clear methods for (i) analyzing and visualizing the density matrix (**DM** or ρ) that describe the spin populations and single- and multiple-quantum coherences (**SQC**s and **MQC**s) and (ii) correlating the influences of FS pulses to changes resulting from evolution. The most common methods for graphically examining such changes involve the plotting of expectation values of spin operators (*i.e.*, $\langle \widehat{\mathrm{O}} \rangle = \mathrm{Tr}\{\rho\widehat{\mathrm{O}}\}$). For instance, a reliable means of visually monitoring the production of transverse spin polarization with a pulse is *via* a plot of $\langle I_x(t) \rangle = \mathrm{Tr}\{\rho I_x(t)\}$, where $\langle I_x(t) \rangle = 0$ indicates maximum transverse spin polarization. It is also possible to render 3D Bloch sphere animations using the quantum toolbox in Python (QuTiP) library, which has pedagogical value for visualization of the time evolution of spin polarization under the influence of unique pulse sequences.

Calculating $\langle I_x(t) \rangle$, $\langle I_y(t) \rangle$, and $\langle I_z(t) \rangle$ will yield the *x*,*y*, and *z* Cartesian coordinates necessary to plot the net nuclear-spin magnetization vector on a 3D Bloch sphere in QuTiP as a function of time. This will be used to monitor the time evolution of spin polarization under irradiation of a WURST pulse in order to visualize the full adiabatic passage process. This will also be used to monitor the build-up of spin polarization under adiabatic WURST irradiation during the BRAIN-CP pulse sequence. Time-dependent expectation values of spin polarization will be calculated using the solid-state simulation software (SIMPSON) and the resulting data will be parsed into the appropriate input format for QuTiP functions. Resulting Bloch-sphere figures will be animated and saved as .gif or .mp4 files for easy visualization *via* the matplotlib library.