**Atlas of Science**
another view on science
https://atlasofscience.org

# What can we achieve for average spin Hamiltonians in solid-state nuclear magnetic resonance spectroscopy?

Multiple-pulse sequences (MPS) have been widely applied in nuclear magnetic spectroscopy to manipulate spin Hamiltonians (such as isolating or enhancing certain interactions while removing the effects of all other interactions), to measure relaxation times, and to enhance the signal. How to effectively manipulate spin Hamiltonians continue to be an important topic, especially in solid-state nuclear magnetic resonance (ssNMR) where various spin Hamiltonians coherently coexist. Ability to select a specific spin Hamiltonian in solid-state systems would allow for simplifying the spin system in order to obtain useful spectroscopic information. In the past several decades, a series of MPS has been developed for homonuclear decoupling, heteronuclear decoupling, multiple quantum excitations, etc., with the aid of a proven powerful theoretical framework – the so-called "average Hamiltonian theory". Recently, the ability to effectively engineer the Hamiltonians is particularly important in quantum computation and quantum simulation, as it is related to the controllability problem of the system. Liquid-state NMR has been recognized as a well-established small-sized qubit quantum information processor to implement the quantum logic gates and simulate quantum dynamics. Due to the complexity of the Hamiltonians and the indistinguishability of nuclear spins in ssNMR, it is more challenging to selectively control the Hamiltonians in solids.

This article considers the problem of how to control the Hamiltonians in solid-state homonuclear NMR systems in the general framework of MPS (Fig. 1). Main results achieved in this paper are as following.

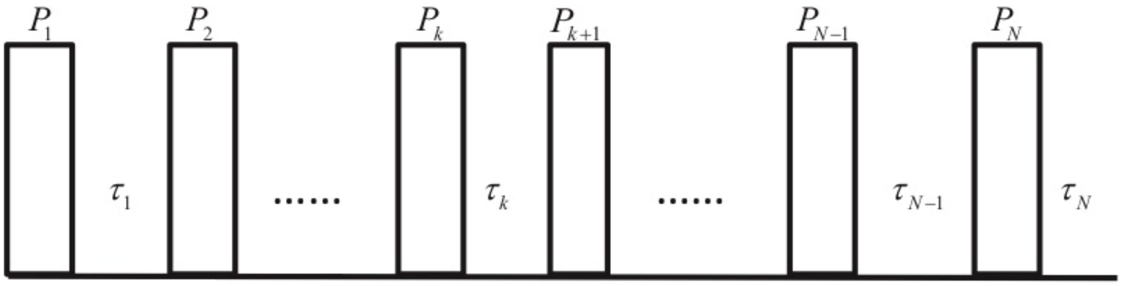

Fig. 1. Framework of a multiple pulse sequence. Here $P_k$ is the *k*th operator for the ideal pulse and $\tau_k$ are time intervals between pulses.

1. We first derived a reachable set of sub-Hamiltonians and developed a general procedure using both flip-angle and phase of applied pulses as control variables under MPS to select any desired sub-Hamiltonian, while suppressing any others, from this reachable set of sub-Hamiltonians.
2. We analyzed the application of homonuclear decoupling and uncovered a new homonuclear decoupling scheme (Fig. 2a). What's the advantage of the new decoupling sequence in comparison with the traditional solid-echo based dipolar decoupling pulse sequences? Well, in the presence of finite pulse length, the new one effectively suppresses the $^1$H–$^1$H homonuclear dipolar interactions while establishes variable scaling factors on the heteronuclear dipolar interactions and chemical shift interactions, depending on the flip-angle of the

applied pulses. When the pulse flip-angle is close to 54.7 °, this sequence possesses a large scaling factor with relatively low average decoupling field. When the pulse flip-angle becomes 120 °, the scaling factor is almost zero, as if forming a "perfect echo". The performance of this new decoupling scheme has been experimentally validated on the crystal sample of $^{15}$N -acetyl-valine (Fig. 2b).

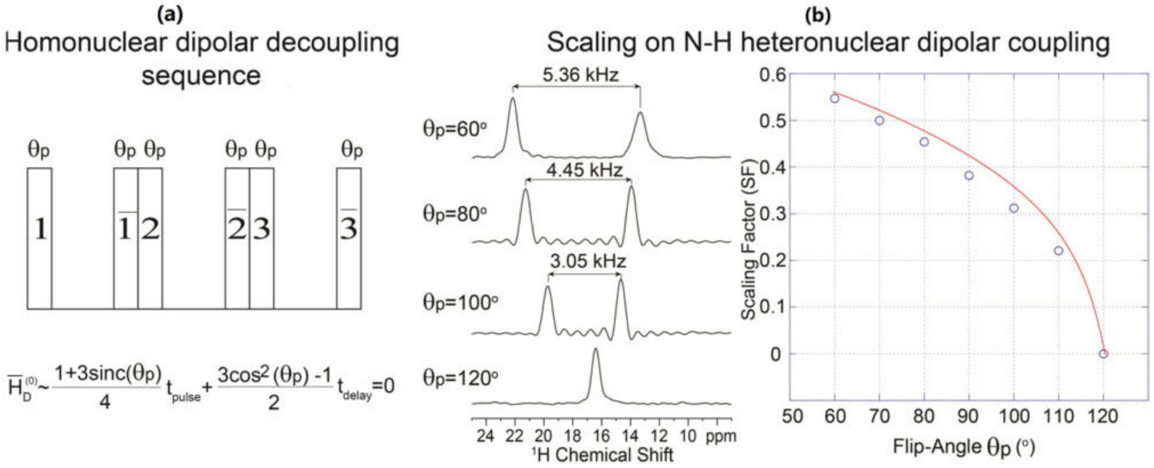

Fig. 2. (a) Basic building block for newly developed homonuclear dipolar decoupling sequence. (b) Experimental performance: the $^{15}$N resonance spectra at 75.4 ppm along the $^{1}$H dimension at different pulse angles and the scaling factor at various pulse flip-angles.

This finding extends our knowledge and ability to engineer spin Hamiltonians in solid-state NMR systems and is expected to have promising applications in the research of solid-state NMR spectroscopy, NMR imaging and NMR quantum computation and quantum simulation.

***Xinhua Peng, Jiangyu Cui, Yuchen Li, Riqiang Fu***
*Department of Modern Physics, University of Science and Technology of China, China*
*National High Magnetic Field Lab, Tallahassee, USA*

## Publication

Engineering spin Hamiltonians using multiple pulse sequences in solid state NMR spectroscopy.
Cui J, Li J, Liu X, Peng X, Fu R
*J Magn Reson. 2018 Sep*