Title:	Understanding Cross-Polarization NMR Experiments Using Multi-Mode Floquet Theory
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Keywords:	Chemistry NMR Magic Angle Spinning Nuclear Magnetic Resonance
Issue Date:	4-Sep-2016
Publisher:	IISER-M
Abstract:	Magic Angle Spinning (MAS) is an important technique routinely employed for obtaining high resolution nuclear magnetic resonance (NMR) spectra in the solid state. In combination with MAS, the cross-polarization (CP) experiment (referred to as CPMAS) forms a vital building block in the design of multi-dimensional solidstate NMR (ssNMR) experiments for studying less sensitive/abundant nuclei. But e cient implementation of CP schemes at faster MAS remains a challenge. Since, the e ciency of CP under MAS depends on intrinsic parameters such as the orientation of the dipolar tensor, magnitude of the chemical shift anisotropy (CSA) interactions and other user control parameters such as the spinning frequency and RF amplitudes, quantitative description of the underlying spin dynamics has always remained elusive. So, along with the development of NMR experiments, re nements in NMR theory are also essential for designing sophisticated experiments and for extracting meaningful constraints from experimental data. To this end, a modi ed version of the CP experiment is proposed employing the concept of eff ective Hamiltonians based on multi-mode Floquet theory. In contrast to other existing schemes in the literature, the proposed schemes could be implemented at higher magnetic fi eld strengths and at faster spinning frequencies. Since bio-molecular applications of solid-state NMR (ssNMR) entail the presence of faster spinning modules, we believe that the design of NMR experiments based on our approach would be benefi cial. Additionally, the mechanism of polarization transfer in CP experiments is described intuitively invoking the phenomenon of dipolar truncation. We believe that the current study would provide the necessary impetus for better design of ssNMR experiments and could be a guiding tool for quantifying the experimental data. The validity of the predictions emerging from our theory is verfii ed with numerical simulations under diff erent experimental conditions.

URI:	http://hdl.handle.net/123456789/683 (http://hdl.handle.net/123456789/683)
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