Abstract

Understanding the response of nuclear spins subjected to an oscillating field has remained an active pursuit in methodology development in NMR spectroscopy. In particular, the response of a quadrupolar nuclear spin (spins with $I > {}^1/_2$) is delicately dependent on the ratio of the quadrupolar coupling constant to the amplitude of the oscillating pulse. In addition to its duration and oscillating frequency. In contrast spin to $I = {}^1/_2$ systems, the time-evolution of the quadrupolar spins during an RF pulse is less understood owing to the dominant presence of the quadrupolar interactions. Consequently, analytic description of the excitation process has remained less transparent within existing theoretical frameworks. As an alternative, the concept of "Effective Floquet Hamiltonians" is explored in the present thesis to explain the nuances of the excitation process in multi-level systems. Employing spin $I = 1$ and ${}^3/_2$ as model systems, a unified theoretical framework for describing the excitation of multiple-quantum transitions in static isotropic and anisotropic solids is proposed within the framework of perturbation theory. The challenges resulting from the anisotropic nature of the quadrupolar interactions are addressed within the effective Hamiltonian framework. The possible role of the various interaction frames on the convergence of the perturbation corrections is discussed along with a proposal for a "hybrid method" for describing the excitation process in anisotropic solids. Employing suitable model systems, the validity of the proposed hybrid method is substantiated through a rigorous comparison between simulations emerging from exact numerical and analytic methods.