Abstract

With the development of technology and improved understanding of nuclear spin-spin interactions and their behavior in static/oscillating magnetic fields, NMR spectroscopy has emerged as a powerful tool for characterizing molecular structure in wide range of systems of chemical, physical and biological relevance. Here in this thesis, employing the concept of effective Hamiltonians, an analytic theory is introduced to describe transitions in a multi-level system in nuclear magnetic resonance (NMR) spectroscopy. Specifically, the discussion is centered towards the treatment of selective and non-selective excitations in static single-crystal and magic angle spinning (MAS) powder sample in quadrupolar spin ($I > 1/2$) systems. Employing the spherical tensor formalism, effective radio-frequency (RF) Hamiltonians are proposed for describing transitions in $I=1$, $3/2$ and $5/2$. The optimum conditions desired for selective excitation in a multi-level system are derived pedagogically from first principles and presented through analytic expressions. As an extension of this approach, multi-quantum (MQ) excitation in quadrupolar systems is discussed. Since MQ NMR spectroscopy of quadrupolar nuclei forms the basis for structural characterization of inorganic solids and clusters, we believe that the analytic theory presented herein would be beneficial both in the understanding and design of MQ NMR experiments.