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Title:	Effective Floquet Hamiltonian theory of multiple-quantum NMR in anisotropic solids involving quadrupolar spins: Challenges and Perspectives
Authors:	Ganapathy, Vinay (/jspui/browse?type=author&value=Ganapathy%2C+Vinay) Ramachandran, Ramesh (/jspui/browse?type=author&value=Ramachandran%2C+Ramesh)
Keywords:	Floquet Hamiltonian multiple-quantum NMR quadrupolar spins
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Abstract:	The response of a quadrupolar nucleus (nuclear spin with $I > 1/2$) to an oscillating radio-frequency pulse/field is delicately dependent on the ratio of the quadrupolar coupling constant to the amplitude of the pulse in addition to its duration and oscillating frequency. Consequently, analytic description of the excitation process in the density operator formalism has remained less transparent within existing theoretical frameworks. As an alternative, the utility of the "concept of effective Floquet Hamiltonians" is explored in the present study to explicate the nuances of the excitation process in multilevel systems. Employing spin $I=3/2$ as a case study, 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.
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