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Title:	On the exactness of effective Floquet Hamiltonians employed in solid-state NMR spectroscopy
Authors:	Garg, Rajat (/jspui/browse?type=author&value=Garg%2C+Rajat) Ramachandran, Ramesh (/jspui/browse?type=author&value=Ramachandran%2C+Ramesh)
Keywords:	Floquet Hamiltonians solid-state NMR spectroscopy
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Abstract:	Development of theoretical models based on analytic theory has remained an active pursuit in molecular spectroscopy for its utility both in the design of experiments as well as in the interpretation of spectroscopic data. In particular, the role of "Effective Hamiltonians" in the evolution of theoretical frameworks is well known across all forms of spectroscopy. Nevertheless, a constant revalidation of the approximations employed in the theoretical frameworks is necessitated by the constant improvements on the experimental front in addition to the complexity posed by the systems under study. Here in this article, we confine our discussion to the derivation of effective Floquet Hamiltonians based on the contact transformation procedure. While the importance of the effective Floquet Hamiltonians in the qualitative description of NMR experiments has been realized in simpler cases, its extension in quantifying spectral data deserves a cautious approach. With this objective, the validity of the approximations employed in the derivation of the effective Floquet Hamiltonians is re-examined through a comparison with exact numerical methods under differing experimental conditions. The limitations arising from the existing analytic methods are outlined along with remedial measures for improving the accuracy of the derived effective Floquet Hamiltonians.
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