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Title:	Understanding multi-quantum NMR through secular approximation
Authors:	Srivastava, Deepansh (/jspui/browse?type=author&value=Srivastava%2C+Deepansh) Venkata Subbarao, R. (/jspui/browse?type=author&value=Venkata+Subbarao%2C+R.) Ramachandran, Ramesh (/jspui/browse?type=author&value=Ramachandran%2C+Ramesh)
Keywords:	Biological relevance Interactions Chemical relevance Physical relevance
Issue Date:	2013
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Citation:	Physical Chemistry Chemical Physics, 15(18), pp.6699-6713.
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 a wide range of systems of chemical, physical and biological relevance. Here in this article, we revisit the important connection between “Secular-Approximation” (a well-known fundamental concept) and NMR spectroscopy. Employing recent experimental results as the background, an alternate interpretation of the secular approximation is presented for describing and understanding the nuances of Multi-Quantum (MQ) NMR spectroscopy of quadrupolar nuclei. Since MQ NMR spectroscopy of quadrupolar nuclei forms the basis of the 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. Additionally, the analytic results are corroborated with rigorous numerical simulations and could be employed in the quantitative interpretation of experimental results.
URI:	<a href="https://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp44296a#!divAbstract">https://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp44296a#!divAbstract</a> ( <a href="https://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp44296a#!divAbstract">https://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp44296a#!divAbstract</a> ) <a href="http://hdl.handle.net/123456789/2919">http://hdl.handle.net/123456789/2919</a> ( <a href="http://hdl.handle.net/123456789/2919">http://hdl.handle.net/123456789/2919</a> )
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