Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Seminar

Effective Hamiltonian and Pulse Design in Solid-state NMR

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The talk will be centred on the theory of experimental methods in solid-state Nuclear Magnetic Resonance (NMR) spectroscopy, which deals with interaction of electromagnetic radiation with nuclei possessing the property of spin, in the presence of a magnetic field. Nuclei with a spin number 1/2 are the focus here. To avoid broad indistinct signals, anisotropic interactions are averaged out by spinning the sample. However, to extract the wealth of information offered by the anisotropic interactions, radio frequency pulses, a control oscillating magnetic field, are applied transverse to the external magnetic field, to recouple the interactions at will, during an experiment. The ones that recouple dipolar interactions form the basis of the talk.

NMR experiments, that involve repeating (periodic) pulse sequences, are generally understood by finding an average or effective Hamiltonian, which approximates the spin dynamics to a great extent and often offers insight into the workings of the experiment that a full numerical simulation of the spin dynamics does not. For average Hamiltonian theory, which can be used to find the effective Hamiltonian, to be applicable for any general pulse sequence with no demands on the different problem frequencies, it is necessary to be able to represent the time-dependent interaction in the Fourier space with finite set of fundamental frequencies, the lack of which is often misunderstood as a limitation of AHT. A formalism to represent the time-dependent interactions in the Fourier space with no more than two frequencies for every involved spin is presented and this enables AHT to be applicable for any pulsed experiment. The formalism has been applied to understand a few established dipolar recoupling pulse sequences. Limitations of the pulse sequences, in particular their sensitivity to isotropic chemical shift, are addressed by designing novel variants of the pulse sequences, aided by insights gained through the effective Hamiltonian description.

Monday, Jan 22nd 2018

02:00 PM (Tea/Coffee at 01:30 PM)

Seminar Hall, TIFR-H