Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Pulse-Sequence Optimisation Based on Effective Floquet Hamiltonians

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Floquet theory is one of the major theoretical frameworks to deal with time-dependent Hamiltonians in magnetic resonance. It is based on a Fourier series expansion of the Hamiltonian that is used to construct an equivalent time-independent but infinite-dimensional representation which is called the Floquet Hamiltonian. While the time-independent Floquet Hamiltonian contains no approximations and leads to the same spectra as the time-dependent Hamiltonian, often an approximative effective Hamiltonian based on perturbation theory is derived. Such effective Hamiltonians based on Floquet theory work well either on or outside resonance conditions but typically do not converge very well near to a resonance condition.

We have recently introduced a new variant of Floquet theory that is based on a continuous Frequency space and not a discrete Fourier series. Such an approach allows us to describe pulse sequences using a finite length of rf irradiation correctly and also describe near-resonance conditions quite well already in a first-order approximation. For such a treatment, the choice of interaction frame becomes important. In our experience, it is often best to include the chemical shift into the interaction-frame transformation to obtain the most accurate description. The calculation of the effective Hamiltonians can be based on single-spin interaction-frame trajectories which makes the calculations computationally quite efficient.

Based on the effective Hamiltonians continuous Floquet theory, we have been implementing a pulse-sequence optimisation strategy. It is based on an effective Hamiltonian optimisation and not on a point-to-point optimisation of the density operator. Therefore, it can take advantage of the single-spin interaction-frame trajectory calculations and does not require a full Hilbert-space simulation. We will show first examples of chemical-shift selective recoupling sequences based on this approach.

Thursday, Jan 25th 2024

14:30 Hrs (Tea / Coffee 14:15 Hrs)

Auditorium, TIFR-H