NMR: From Strong-Correlation to Life Sciences

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Nuclear Magnetic Resonance (NMR) is one of the most important tools for the structure analysis of molecules and a widely used technique in chemical and pharmaceutical industry. I briefly introduce our approach to calculate NMR spectra starting from the SMILES description or just the name of the molecule. To this end we first determine the 3D structure of the molecule from which we obtain the NMR spin Hamiltonian after averaging over conformers and rotamers. The resulting NMR Hamiltonian is a Heisenberg Hamiltonian with site dependent magnetic fields (chemical shifts). Although this Hamiltonian is strongly correlated, the corresponding NMR spectral functions can be calculated using a clustering approach due to the large gyromagnetic rations of the relevant nuclei.

Recently we enhanced our NMR simulation techniques to perform an automatic adaption of the obtained NMR parameter to experimental data. Using this technique we can determine accurate reference parameter for NMR spectra.

In a next step we are using these reference parameter to extract the concentration of compounds from the NMR spectrum of mixtures for example for applications in metabolomics like the analysis of urine and blood.

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[1] Fratus et al., “Can a Quantum Computer Simulate Nuclear Magnetic Resonance Spectra Better than a Classical One?”, arXiv:2508.06448