J-coupling NMR Spectroscopy with Nitrogen Vacancy Centers at High Fields [1]

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A diamond-based sensor utilizing nitrogen-vacancy (NV) center ensembles permits the analysis of micron- sized samples through NMR techniques at room temperature [2]. Current efforts are directed towards extending the operating range of NV centers into high magnetic fields, driven by the potential for larger nuclear spin polarization of the target sample and the presence of enhanced chemical shifts. Especially interesting is the access to J-couplings as they carry information of chemical connectivity inside molecules [3]. In this work, we present a protocol to access J-couplings in both homonuclear and heteronuclear cases with NV centers at high magnetic fields. Our protocol leads to a clear spectrum exclusively containing J-coupling features with high resolution. This resolution is limited primarily by the decoherence of the target sample, which is mitigated by the noise filtering capacities of our method.

References

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[3] M. H. Levitt, *Spin Dynamics: basics of Nuclear Magnetic Resonance, 2nd ed.* (Wiley, Chichester, 2008)

[4] C. Munuera-Javaloy, A. Tobalina, and J. Casanova, Physical Review Letters, **130** (2023) 13360

Figures

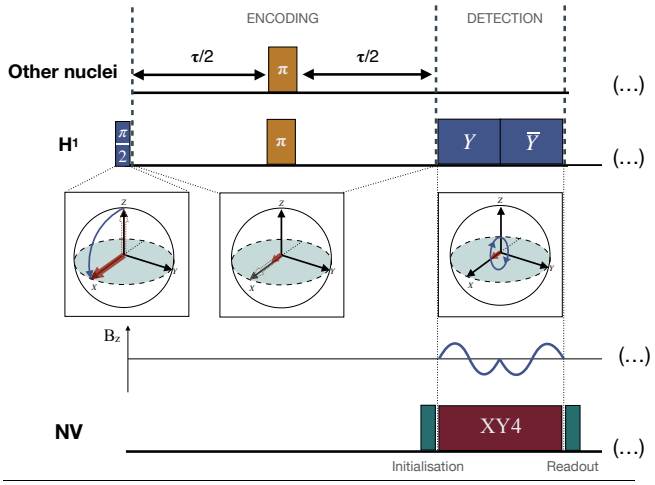

Figure 1: Scheme of one step of the protocol. The sequence begins by driving the hydrogen nuclei to the |+> state. By employing a free evolution interval τ, with by a π-pulse at its midpoint, we selectively isolate the desired J-couplings while simultaneously mitigating the impact of magnetic field inhomogeneities. This approach effectively extends the coherence time of the sample from T2* to T2. Then, the signal emitted by the sample (proportional to the magnetisation, depicted bellow the sequence) is read via an heterodyne read-out protocol [4] with the nitrogen vacancy center ensemble.

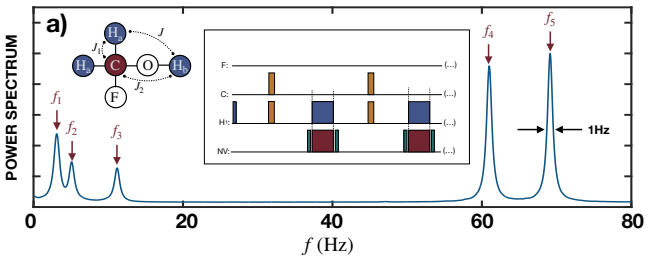

Figure 2: Simulation of the protocol using fluoromethanol as the target molecule. The obtained peaks in the Fourier space are directly related to the couplings depicted in the scheme of the molecule. In this case, only the coupling among hydrogens and carbons are targeted (as well as those between non-equivalent hydrogens). The frequency resolution is estimated to be approximately 1Hz, which is about 3 times better than when working with T2*.