Nuclear Spin Qudits for Quantum Algorithms

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Abstract: Molecules with hyperfine-coupled electronic and nuclear spins are shown to be promising platforms for qudit-based quantum algorithms implemented with NMR pulse sequences

Molecular nanomagnets (MNMs), molecules containing one or few interacting spins, are emerging as promising building blocks for quantum technologies [1]. Since they naturally provide many accessible low-energy levels, they are particularly suitable to encode qudits, i.e. quantum digits with more than 2 levels, thus enlarging the tools of quantum logic with respect to qubit-based architectures. For instance, MNMs containing single metal ions with a non-zero nuclear spin, strongly coupled to the electronic one by a large hyperfine interaction, can provide a significant number of states for qudit-based algorithms. Their sizable hyperfine interaction on the one hand, enables thermal initialization by cooling below ~10 mK, on the other, it makes nuclear spin manipulations by radio-frequency pulses much faster.

^{173}Yb(trensal) provided the first example of a nuclear qudit system, which can be rapidly and coherently manipulated with NMR pulses. Here we show that by exploiting a sub-manifold of the Yb(trensal) energy spectrum, we successfully realized the first proof-of-concept quantum simulator based on molecular qudits manipulated with a flexible broadband NMR spectrometer [2,3].

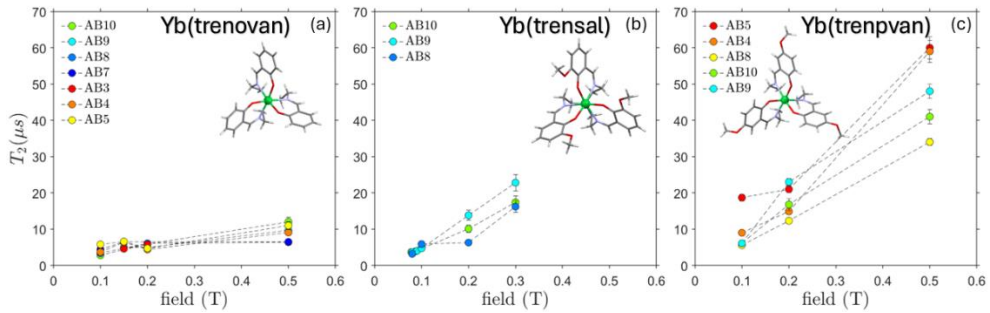

Fig. 1 Coherence time T_2 for nuclear transitions of Yb(trenovan) (panel a), Yb(transal) (panel b), Yb(trenpvan) (panel c) measured at T =1.4 K as a function of the applied magnetic field applied orthogonal to the molecular C_3 symmetry axis. Molecular structure are shown as inset.

New molecular qudits, derived from the parent compound Yb(transal), were also investigated with NMR: Yb(trenpvan) and Yb(trenovan) (Fig. 1). Despite their very similar molecular structure, the three compounds show different temperature and magnetic field dependence of the coherence times T_2. We also demonstrated that their coherence times can be further increased by employing a CPMG pulse sequence, i.e. a concatenation of *n* refocusing pulses to dynamically decouple the system from the environment. New multi-frequency experiments on the Yb(trenpvan) are currently underway, with the aim to implement quantum algorithms such as the Quantum Fourier Transform, also exploiting the recently developed double-frequency SEDOR NMR probe.

All these characterizations and proof-of-principle experiments will also be performed exploiting the custom-designed dilution refrigerator, soon-to-be delivered at the University of Parma. This new apparatus, reaching temperatures below 10 mK, is also equipped with a dedicated tunable NMR probe working in the 10 MHz-1 GHz range. With this experimental upgrade, investigation of decoherence at very-low temperatures and thermal initialization of nuclear spin qudits will finally become possible.

References

[1] A. Chiesa, P. Santini, E. Garlatti, F. Luis and S. Carretta, "Molecular nanomagnets: a viable path toward quantum information processing?", Rep. Prog. Phys. **87**, 034501 (2024).
[2] S. Chicco, G. Allodi, A. Chiesa, E. Garlatti, C. D. Buch, P. Santini, R. De Renzi, S. Piligkos, S. Carretta, "Proof-of-concept Quantum Simulator based on Molecular Spin Qudits", J. Am. Chem. Soc. **146**, 1053–1061 (2024).
[3] G. Allodi, A. Banderini, R. De Renzi, C. Vignali, Rev. Sci. Instrum. **76**, 083911 (2005).