Understanding decoherence in molecular spin qudits

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Molecular nanomagnets are quantum spin systems that, thanks to their many accessible low-energy states, potentially serve as qudits for future quantum technologies [1]. At low temperatures, the primary source of error in these systems is pure dephasing, caused by their interactions with the bath of surrounding nuclear spins degrees of freedom. Most importantly, as the system's dimensionality grows going from qubits to qudits, the control and mitigation of decoherence become more challenging. Here, we analyze the characteristics of pure dephasing in molecular qudits under spin-echo sequences. We use a realistic description of their interaction with the bath, whose non-Markovian dynamics is accurately computed by the cluster correlation expansion technique [2]. First, we analytically show that the differences in the expectation values of the local spin operators on the eigenstates of the qudit are the source of decoherence in these systems. Indeed, we demonstrate that this is a necessary and sufficient condition to prevent the decay of coherence with time, also introducing a parameter to quantify the deviation from such an ideal condition. We illustrate this with two paradigmatic systems: a single giant spin and a composite antiferromagnetic spin system. We then advance a proposal for optimized nanomagnets, identifying key ingredients for engineering robust qudits for quantum technologies [3].

References

[1] Alessandro Chiesa, Paolo Santini, Elena Garlatti, Fernando Luis and Stefano Carretta, Reports on Progress in Physics, 87(2024) 034501
[2] Wen Yang, Ren-Bao Liu, Physical Review B, 78 (2008) 08531
[3] Leonardo Ratini, Giacomo Sansone, Elena Garlatti, Francesco Petiziol, Stefano Carretta, Paolo Santini, Physical Review Research, 4 (2025), 043125

Figures

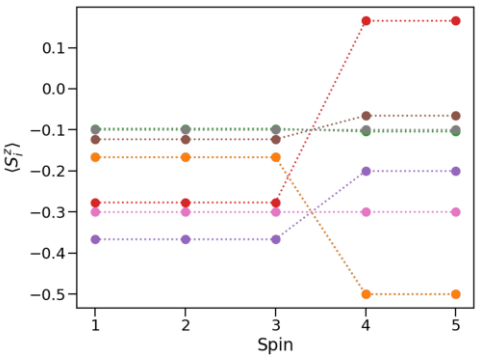

Figure 1: Expectation values of the local spin operators for selected eigenstates of a system composed of 5 spins, interacting through antiferromagnetic interactions.

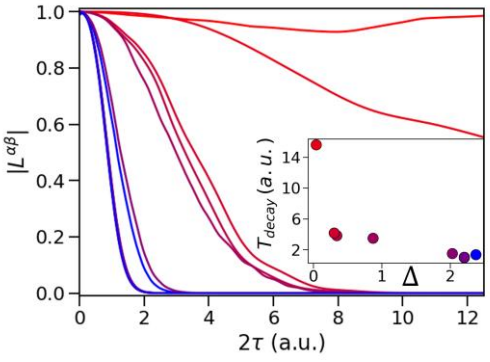

Figure 2: Coherence factor curves for the superposition of selected eigenstate pairs (arbitrary time units). Inset: Decay time as a function of the parameter.