

Molecular spin qudits to test generalized Bell inequalities

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Abstract: We show that molecular nanomagnets provide an ideal platform to probe generalized Bell inequalities on qubit-qudit and qudit-qudit pairs, demonstrating robust violation through optimized pulse sequences and realistic simulations based on experimentally measured parameters.

Bell inequalities [1] are the standard tool to certify quantum correlations and rule out local hidden-variable models. While extensively tested on qubits, the extension to qudits - systems with dimension greater than 2 - remains largely unexplored, despite the advantages that high-dimensional encodings offer over standard qubits [2]. Molecular nanomagnets (MNMs) are a suitable platform to test generalized Bell inequalities on qudits, combining a well-defined multilevel spin structure with long coherence times and chemically tunable interactions [2].

Here we propose to investigate the violation of the Clauser-Horne-Shimony-Holt (CHSH) inequality in the molecular system $^{173}\text{Yb}(\text{trensal})$. In this case, entanglement is established between a qubit encoded in the electronic spin and a qudit encoded in the nuclear spin 5/2. By leveraging the intrinsic multidimensionality of the system, we demonstrate correlations in a state that cannot be trivially reduced to a standard qubit-qubit entangled state by numerical simulations using experimentally measured parameters and including the full pulse sequence and decoherence (Fig.1 (left)).

Our second proposal focuses on testing the CGLMP inequality [3] in a realistic spin-3/2–spin-3/2 system, where a switchable interaction between two qudits is realized through the inclusion of an interposed qubit. This setup allows for the generation of entangled states between the two qudits, which can then be brought to a non-interacting regime once their interaction is switched off [2]. This is ideal for probing Bell inequalities and exploits the unique properties of molecular nanomagnets, using realistic parameters suitable for a proof-of-principle experiment (Fig 1 (right)).

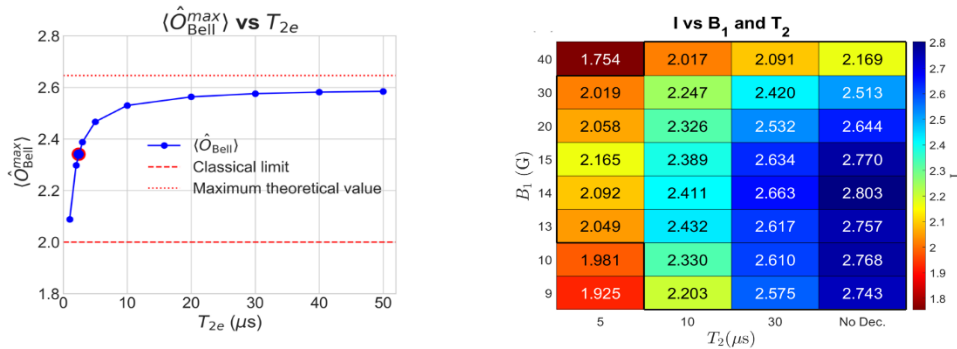


Fig. 1 (Left) Maximum expectation value of the CHSH Bell operator ($\langle \hat{O}_{\text{Bell}}^{\text{max}} \rangle$) as a function of decoherence time T_{2e} for the $^{173}\text{Yb}(\text{trensal})$ qubit-qudit system. The red dashed line marks the classical limit; the red circle indicates the experimentally measured T_{2e} . (Right) CGLMP functional I as a function of driving field amplitude B_1 and dephasing time T_2 for the spin-3/2–spin-3/2 molecular trimer. Violation of the CGLMP inequality ($I > 2$) is obtained across a wide range of realistic parameters.

Our study highlights the potential of molecular nanomagnets as scalable platforms for investigating high-dimensional quantum correlations and contributes to the broader exploration of qudits in quantum information, sensing, and simulation technologies [4].

References

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