

Molecular spin qudits to test generalized Bell inequalities

Silvia Macedonio ^{1,2} Luca Lepori,^{1,2} Alessandro Chiesa ^{1,2,3} Simone Chicco ¹ Laura Bersani ¹
 Marcos Rubin-Osanz,¹ Lukas Bradley Woodcock ⁴ Athanasios Mavromagoulos,⁴ Giuseppe Allodi ¹
 Elena Garlatti ^{1,2,3} Stergios Piligkos ⁴ Augusto Smerzi ⁵ and Stefano Carretta ^{1,2,3,*}

¹*Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Parco Area delle Scienze, 7/A, I-43124 Parma, Italy*

²*Gruppo Collegato di Parma, INFN-Sezione Milano-Bicocca, I-43124 Parma, Italy*

³*UdR Parma, INSTM, I-43124 Parma, Italy*

⁴*Department of Chemistry, University of Copenhagen, DK-2100 Copenhagen, Denmark*

⁵*QSTAR and INO-CNR and LENS, Largo Enrico Fermi 2, 50125 Firenze, Italy*



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We show that molecular nanomagnets provide an ideal platform to investigate entanglement in qubit-qudit and qudit-qudit pairs. A prototypical example is ^{173}Yb (trensai), embedding an electronic spin qubit coupled to a nuclear spin qudit. We demonstrate violation of generalized Bell inequalities on this molecule by developing an optimized pulse sequence and by performing realistic numerical simulations using experimentally measured Hamiltonian parameters and coherence times. We find that the inequalities are safely violated in a wide range of parameters, proving the robustness of entanglement in the investigated system. Furthermore, we propose a scheme to study qudit-qudit entanglement on a molecular spin trimer, in which two spins $3/2$ are linked via an interspersed switch to turn on and off their mutual interaction.

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I. INTRODUCTION

Entanglement is a cornerstone of quantum technologies, enabling critical advancements in quantum computing, cryptography, and sensing by exploiting quantum correlations for tasks that are impossible with classical systems [1–3]. The characterization of these correlations is an increasingly relevant problem for both foundational investigations and for the advancement of quantum technologies. This is usually done by preparing an entangled state of two objects and then measuring local observables on the two subsystems. The results are then combined to test the so-called Bell inequalities, whose violation represents a signature of quantum correlations and is generally used as a benchmark for distinguishing quantum predictions from local hidden-variable (HV) models [4].

So far, most experimental and theoretical efforts to verify Bell inequalities have focused on qubit systems [5,6]. The extension to qudits remains mostly unexplored, despite the growing availability of them in platforms like molecular nanomagnets, trapped ions, Rydberg atoms, transmons [7–11], as well as the increasing interest for qudit-based encodings for quantum simulation, sensing, and computation. Indeed, unlike traditional qubits, hosting only two states, qudits have the capability to encode quantum information across multiple

states, providing a larger Hilbert space per physical unit that can enhance computational power, increase information density, and improve resistance to errors [12,13]. For instance, they allow more compact encodings with reduced number of entangling gates for quantum computation [14] or quantum simulation [15–18] and can embed quantum error correction within single objects [19–22], greatly simplifying its actual implementation. Moreover, high-dimensional systems have shown significant advantages in quantum key distribution and quantum communication, where they can enhance security, robustness against noise, and channel capacity [23,24].

From a foundational perspective, qudit entanglement is not merely a higher-dimensional analog of qubit entanglement: it supports qualitatively different forms of nonclassical correlations. In this context, generalized Bell inequalities for d -dimensional systems serve as useful tools for validating genuine high-dimensional entanglement [5,25,26]. Moreover, similar to the qubit case, they are sufficient to verify the Kocken-Speker contextuality of hidden-variable models of quantum mechanics [27]. This property is considered a crucial resource for quantum computation advantages [28,29]. Probing generalized Bell inequalities on qudits is therefore important for both fundamental and applicative issues. However, finding a suitable platform for that task is not trivial, especially due to the intrinsic difficulty in the coherent manipulation of multilevel systems.

A convenient experimental platform providing qudits with even large spin-manifold dimensions is offered by molecular nanomagnets (MNM) [10]. These solid-state systems have gained considerable attention as building blocks for qudit-based quantum information processing due to their unique characteristics. In particular, the long coherence times [30] and versatile spin dynamics of MNMs enable precise control

*Contact author: stefano.carretta@unipr.it

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and manipulation of these qudits [31,32]. Moreover, microscopic interactions, level structure, eigenstates, and coherence properties of MNMs can often be tuned at the synthetic level to a large extent [33–37]. This allows to leverage the multi-level structure of MNMs for robust error correction schemes and efficient implementation of quantum algorithms, e.g., for quantum simulation and sensing [10,15,16,22,38–41].

Here, we propose the use of the ^{173}Yb (trensai) MNM to test generalized Bell inequalities on spin qudits. This system provides an effective electronic spin 1/2 coupled by a strong hyperfine interaction to a nuclear spin 5/2, showing remarkably long coherence times. Such a qubit-qudit pair represents the simplest setup to test Bell inequalities beyond the qubit-qubit case. In particular, we focus on four qudit levels and we propose a largely device-independent protocol for the experimental verification of the Clauser-Horne-Shimony-Holt (CHSH) generalized Bell inequality on this $(\frac{1}{2}-\frac{3}{2})$ molecular spin dimer, only relying on a few basic and standard assumptions, like fair sampling [42] and measurement independence [43–48]. We design the sequence of pulses to generate entangled states and then to perform local unitary transformations before measuring expectation values on the two spins. We characterize the system by measuring its electronic and nuclear spin coherence times in a highly diluted sample. We then use these values to numerically simulate experiments to probe the considered inequalities. The gradient ascent pulse engineering (GRAPE) algorithm [49] is exploited to optimize the sequence and thus reduce the leakage and/or the pulse duration, thus greatly mitigating the effect of decoherence. As a result, we obtain very high fidelity and we demonstrate the violation of the CHSH inequalities using experimentally measured Hamiltonian parameters and coherence times and experimentally feasible pulses. We adopted four-level qudits since this minimal choice is the ideal one to design a proof-of-concept experiment. Indeed, we checked that it allows for significant violations of CHSH inequality. Moreover, working with an effective spin-3/2 system keeps the number of control pulses manageable, which is essential for an efficient implementation: Shorter sequences reduce the impact of decoherence and other noise sources during the manipulation. Increasing the qudit dimension would require substantially longer pulse sequences, making the experimental realization significantly more susceptible to imperfections.

In addition, we extend our protocol to two entangled qudits, such as a molecular spin $(\frac{3}{2}-\frac{3}{2})$ dimer. In this case, we evaluate the Collins-Gisin-Linden-Massar-Popescu (CGLMP) inequality [50], explicitly designed for pairs of d -dimensional systems [51].

Demonstrating Bell-type correlations in such systems, under realistic conditions and including the effects of decoherence, provides both a meaningful test of quantum mechanics and a benchmark for future applications in quantum simulation, metrology, semi-device-independent certification and error-corrected computation.

II. CHSH INEQUALITY FOR A $(\frac{1}{2}-\frac{3}{2})$ SYSTEM

The general formalism for CHSH-type inequalities on a qubit-qudit pair has been recently developed in Ref. [52], generalizing the results obtained for qubit-qubit systems [53].

Indeed, it was previously shown [54] that dichotomic measurements at the basis of the CHSH formalism are sufficient to probe the validity of hidden-variables statistical models also on qubit-qudit states. The net effect is that these models can be efficiently probed on qubit-qudit states by properly redefined CHSH inequalities.

In this context, each subsystem is assigned to a party—commonly referred to as “Alice” and “Bob”—who can perform one of two measurements on the respective subsystem. We denote by A and A' the two observables measured by Alice (on the qubit), and by B and B' the two observables measured by Bob (on the qudit). These measurements are repeated on multiple copies of the system to estimate the probabilities of the various joint outcomes [51,55]. To test local HV models, one considers the expectation value of the Bell operator

$$\hat{O}_{\text{Bell}} = A \otimes (B + B') + A' \otimes (B - B'), \quad (1)$$

where A, A' and B, B' are Hermitian observables with eigenvalues $\{+1, -1\}$. This operator form follows from

$$|E(a, b) - E(a, b') + E(a', b) + E(a', b')| \leq 2,$$

by expressing the four correlations as expectation values of tensor-product observables, $E(a, b) = \langle A \otimes B \rangle$, and using linearity of the expectation value, together with the symmetry of the CHSH functional under relabelling of measurement settings (see Ref. [52] and the Supplemental Material [56]). A violation of the CHSH inequality, excluding the possibility of a local HV description, occurs whenever

$$\langle \psi | \hat{O}_{\text{Bell}} | \psi \rangle > 2, \quad (2)$$

for a composite quantum state $|\psi\rangle$. Such a violation reveals the presence of nonclassical correlations and hence the genuinely quantum nature of the joint qubit-qudit state $|\psi\rangle$. We focus hereafter on the following entangled qubit-qudit state for a spin $(\frac{1}{2}-\frac{3}{2})$ dimer:

$$|\psi\rangle = \frac{1}{2} \left(\left| \uparrow, \frac{3}{2} \right\rangle + \left| \uparrow, -\frac{1}{2} \right\rangle + \left| \downarrow, -\frac{1}{2} \right\rangle + \left| \downarrow, -\frac{3}{2} \right\rangle \right), \quad (3)$$

which is constructed to be non-reducible to a spin $(\frac{1}{2}-\frac{1}{2})$ state via local unitary operations on the qudit (see the Supplemental Material [56]). This guarantees that we exploit the full qubit-qudit structure. For this state, we numerically determine the observables A, A', B, B' that maximize the violation of the Bell inequality, yielding a theoretical upper bound:

$$\langle \psi | \hat{O}_{\text{Bell}} | \psi \rangle = 2.64575. \quad (4)$$

This benchmark sets the maximum violation achievable in our scenario and is used to evaluate the results of the implemented protocol.

III. MOLECULAR SPIN DIMER TO TEST CHSH INEQUALITY

The entangled state $|\psi\rangle$ in Eq. (3) can be experimentally realized using ^{173}Yb (trensai) [57], which hosts an electronic effective spin 1/2 coupled by hyperfine interaction to a nuclear spin 5/2. We exploit the electronic spin to encode the qubit and four nuclear spin states to encode the spin-3/2 qudit. The

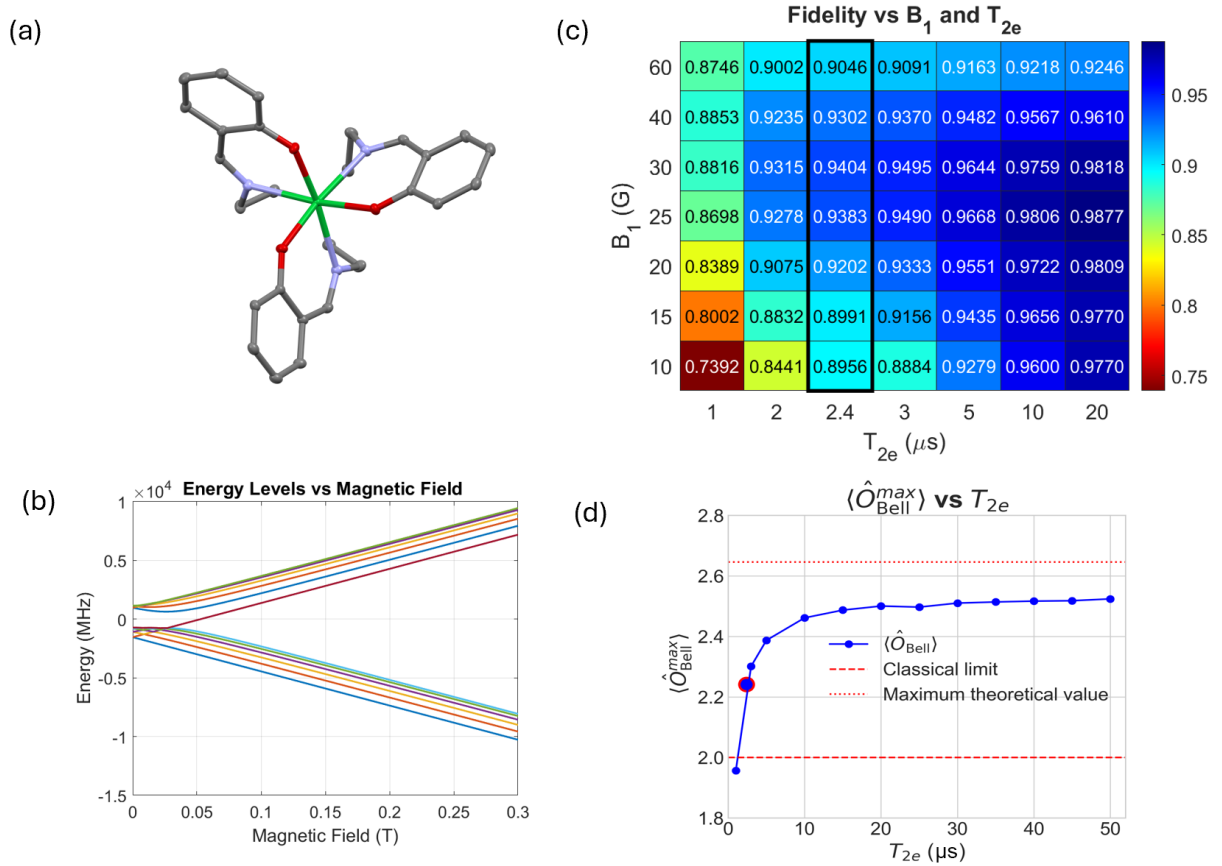


FIG. 1. (a) Molecular structure of ^{173}Yb (trensall). Color scheme: C (gray), O (red), N (blue), Yb (green). H atoms have been omitted for clarity. (b) Energy level diagram of the electronuclear states of ^{173}Yb (trensall) as a function of the static magnetic field B_0 along z axis. The system provides an $S = 1/2 - I = 5/2$ spin pair coupled by hyperfine interaction, used to probe CHSH inequality for $B_0 = 0.3 \text{ T}$. (c) Fidelity $\mathcal{F}$ as a function of control field amplitude B_1 and decoherence time T_{2e} in the preparation of the entangled state $|\psi\rangle$. The black box marks the experimentally measured T_{2e} . (d) $\langle \hat{O}_{\text{Bell}}^{\text{max}} \rangle$ as a function of decoherence time T_{2e} , starting from the optimal entangled states. Violation of the CHSH inequality is obtained for $\langle \hat{O}_{\text{Bell}}^{\text{max}} \rangle > 2$ (red dashed line).

molecule is shown in Fig. 1(a) and described by the following Hamiltonian:

$$H = g_S \mu_B B_z S_z + g_I \mu_N B_z I_z + A_{\perp} (S_x I_x + S_y I_y) + A_{\parallel} S_z I_z + p I_z^2, \quad (5)$$

where $g_S = (2.9, 2.9, 4.3)$ represents an anisotropic electronic g factor, $g_I = -0.2592$ is the nuclear g factor, $A_{\parallel} = -883 \text{ MHz}$ and $A_{\perp} = -628 \text{ MHz}$ are the hyperfine coupling constants along the z axis and in the perpendicular plane, respectively, and $p = -66 \text{ MHz}$ represents the axial nuclear quadrupole interaction. A level diagram as a function of the external field is reported in Fig. 1(b). Hereafter, we consider an external static magnetic field $B_z = 0.3 \text{ T}$ applied along the z axis. At this field, the eigenstates are practically factorized into electronic and nuclear spin components and hence represent the good starting point to test CHSH inequalities. Nonetheless, a tiny electronuclear mixing of the wavefunction yields a sizable enhancement of the matrix elements of nuclear spin transitions, enabling fast manipulations of the nuclear states. At this optimized magnetic field, we experimentally characterize the electronic and nuclear spin coherence of the system by pulsed Electron Paramagnetic Resonance (EPR) and broadband Nuclear Magnetic Reso-

nance (NMR). Measurements are performed on single crystal of ^{173}Yb (trensall) at 0.05% dilution—the best compromise for having a strong enough echo signal and negligible intermolecular dipolar interactions. The results are shown in the Supplemental Material along with additional experimental details [56]. The nuclear coherence time T_{2n} was measured for four transitions among the hyperfine levels of Yb (trensall) and fitted to an exponential function, consistently with the Lindblad master equation used in our numerical simulations (vide infra). We find remarkably long values ($\gtrsim 500 \mu\text{s}$) for all transitions. In the simulations below, we considered the shortest $T_{2n} = 560 \mu\text{s}$ obtained from these fits, in order to include the effect of pure dephasing in the less favorable conditions.

The electronic spin coherence time in the same conditions of dilution and external field was measured by pulse EPR, resulting in $T_{2e} \sim 2.4 \mu\text{s}$ at 2.7 K (see the Supplemental Material [56]).

IV. PULSE SEQUENCE AND DEMONSTRATION OF VIOLATION OF THE CHSH INEQUALITY

The target state $|\psi\rangle$ in Eq. (3) is obtained starting from the ground state $|\downarrow, -\frac{5}{2}\rangle$ of the Hamiltonian in Eq. (5) and applying suitable sequences of electromagnetic pulses to implement

single-qubit, single-qudit, and joint qubit-qudit gates [10] (see the Supplemental Material for details [56]). These are realized via resonant square pulses, whose frequency and duration define which transition is addressed and the rotation angle. Numerical simulations of the whole pulse sequence, including the effect of pure dephasing, are performed by solving the Lindblad master equation:

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_j \gamma_j \left(L_j \rho L_j^\dagger - \frac{1}{2} \{L_j^\dagger L_j, \rho\} \right), \quad (6)$$

where γ_j denotes the dephasing rate acting on site j and L_j are the corresponding jump operators [58]. At low temperatures, these systems exhibit very long relaxation times and pure dephasing is by far the dominant noise effect [59,60]. Hence, the relevant jump operators in Eq. (6) are S_z and I_z with corresponding rates $\gamma_j = 1/T_{2e}$ and $1/T_{2n}$.

At the end of the simulation, we compute the fidelity $\mathcal{F} = \langle \psi | \rho | \psi \rangle$ between the final density matrix ρ and the target state. The fidelity is optimized by tuning the pulse amplitude B_1 , balancing spectral selectivity and decoherence. Indeed, the pulse duration is proportional to $1/B_1$ and hence increasing B_1 on the one hand reduces the effect of decoherence, on the other hand can yield leakage toward transitions occurring at similar frequencies. In particular, we obtain $|\psi\rangle$ through five pulses: one microwave addressing a qubit transition for a specific nuclear spin state and four radiofrequency pulses addressing nuclear spin transitions.

To optimize the pulse sequence and test its robustness to noise, we have studied the fidelity in the construction of $|\psi\rangle$ as a function of B_1 and of the coherence times. First, we note that experimentally measured values of T_{2n} are much longer than the pulse sequence duration, typically lasting 0.5–1 μ s for the optimal B_1 . Hence, we fixed T_{2n} at the experimentally measured value of 560 μ s and compute $\mathcal{F}$ as a function of T_{2e} and B_1 . By proper choice of B_1 , fidelities above 0.95 were obtained for all values of T_{2e} . Results are shown in Fig. 1(c); in particular, in the construction of the entangled state $|\psi\rangle$, for all decoherence scenarios a maximum appears and shifts to higher B_1 as T_{2e} decreases. In particular, a fidelity above 0.94 is obtained using the measured $T_{2e} = 2.4 \mu$ s [highlighted by a thick box in Fig. 1(c)].

The expectation value of the Bell operator in Eq. (1) can be equivalently reformulated in terms of a more experimentally accessible set of four expectation values of diagonal spin operators, S_z for the qubit and D_j for the qudit, after rotating the state via local unitaries [61]. It can thus be expressed as

$$\langle \psi | \hat{O}_{\text{Bell}}^{(\max)} | \psi \rangle = O_{11} + O_{12} + O_{21} - O_{22}, \quad (7)$$

where each O_{ij} corresponds to a joint measurement on the rotated state $\rho_{A_i, B_j} = (U_{A_i} \otimes U_{B_j}) |\psi\rangle \langle \psi| (U_{A_i}^\dagger \otimes U_{B_j}^\dagger)$, with $i, j = 1, 2$. The four expectation values are

$$O_{ij} = \text{Tr}[(-2S_z \otimes D_j) \rho_{A_i, B_j}], \quad (8)$$

with

$$D_1 = \text{diag}(-1, 1, 1, 1), \quad D_2 = \text{diag}(1, -1, 1, 1). \quad (9)$$

Direct implementation of the unitary operations $(U_{A_i} \otimes U_{B_j})$ via hand-optimized pulses yielded insufficient fidelities due to large leakage. To overcome this, we employed GRAPE

optimization [49,62,63], which designs optimal control pulses by discretizing control fields into N time segments, each with constant amplitude. The procedure dynamically optimizes the control fields via gradient ascent maximization of the process fidelity $\mathcal{F}_U = |\langle U_{\text{target}} | U(T) \rangle|^2$ between the target unitary $U_{\text{target}} = U_A \otimes U_B$ and the computed time-evolution operator $U(T)$ (see the Supplemental Material [56]). In this way, high-fidelity quantum operations can be achieved, balancing computational efficiency and experimental robustness [64–66]. The control fields were constrained to experimentally realistic values of the amplitudes (maximum $B_1 = 7.5$ mT) and the frequencies (not exceeding 800 MHz), consistent with typical NMR conditions. Within these realistic boundaries, the protocol successfully prepares each of the four rotated states ρ_{A_i, B_j} in a time of approximately 1 μ s. Remarkably, we obtain values of $\langle \hat{O}_{\text{Bell}}^{(\max)} \rangle$ that consistently violate the Bell inequality across all tested decoherence regimes [dashed red line in Fig. 1(d)] and in particular for $T_{2e} = 2.4 \mu$ s (red circle). These results demonstrate the robustness of the observed quantum correlations in our qubit-qudit platform in a realistic simulation of the experimental protocol. Remarkably, the scheme for demonstrating violation of CHSH inequalities does not require projective measurements but only ensemble expectation values. All in all, these findings pave the way to an actual implementation of the procedure with a broadband nuclear magnetic resonance setup on available molecular crystals of ^{173}Yb (trensall).

V. EXTENSION TO A TWO-QUDITS DIMER

In the previous proof-of-concept experiment, the coupling between the two parties was always on, although ineffective in the proposed working conditions. We now propose an alternative platform in which the entanglement between the qudits is turned on and off when required, through a switchable coupling mechanism mediated by a spin-1/2 ancilla [10]. In principle, this system can allow spacelike separation. Moreover, we now explore a fully symmetric two-qudit configuration, focusing on an entangled state of two spin-3/2 qudits. A possible realization of this $(\frac{3}{2} - \frac{1}{2} - \frac{3}{2})$ molecular spin trimer is represented by two Cr^{3+} ions in a distorted octahedral environment ($S = 3/2$) [67], linked through an interleaved Yb (trensall) [41,68]. If we only consider the electronic spin degrees of freedom, the latter behaves at low energy as an effective spin doublet. The spin Hamiltonian of the system (sketched in Fig. 2) is

$$\begin{aligned} \mathcal{H} = & \mu_B B_z (g_1^z S_1^z + g_2^z S_2^z + g_3^z S_3^z) \\ & + J_{12} (S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z) \\ & + J_{23} (S_2^x S_3^x + S_2^y S_3^y + S_2^z S_3^z) \\ & + D_1 S_1^{z^2} + D_3 S_3^{z^2}, \end{aligned} \quad (10)$$

where S_i^α , $\alpha = (x, y, z)$, is a spin-1/2 operator associated ancilla and S_i^α , $i = 1, 3$ is a spin-3/2 operator. An external magnetic field $B_z = 1.3$ T is applied along the z axis, activating the Zeeman terms, which are proportional to $\mathbf{g}_1 = (2.0, 2.0, 2.0)$, $\mathbf{g}_2 = (2.9, 2.9, 4.3)$, and $\mathbf{g}_3 = (1.95, 1.95, 1.95)$, respectively. Additionally, the system includes two isotropic exchange terms, $J_{12} = 5 \times 10^{-3}$ meV

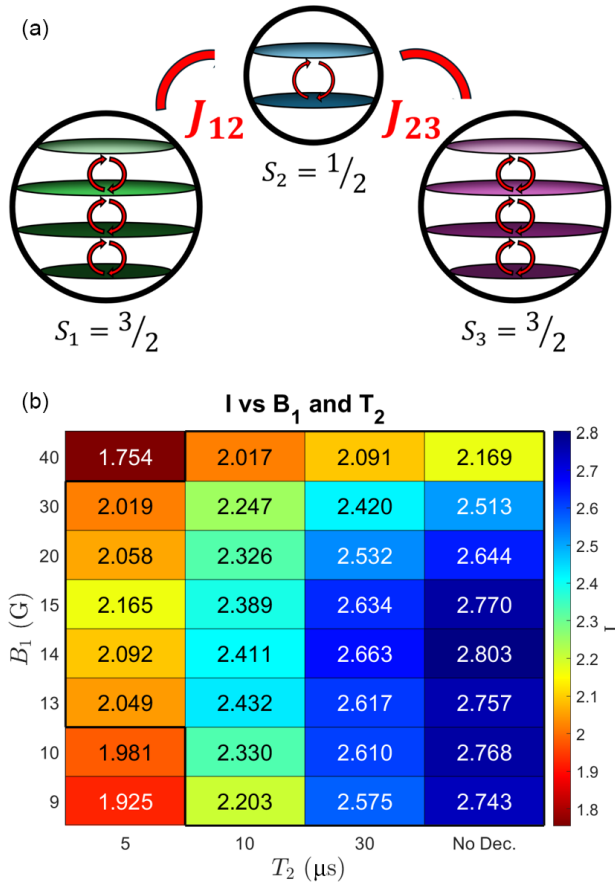


FIG. 2. (a) Schematic representation of the molecular spin trimer proposed to test CGLMP inequality on a pair of four-level qudits. It consists of two spin-3/2 qudits (S_1, S_3) coupled via isotropic exchange interactions J_{12}, J_{23} to a two-level switch (S_2). A static magnetic field $B_0 = 1.3$ T is applied along the z direction. (b) Value of the Bell functional I as a function of the driving field amplitude B_1 and of the dephasing time T_2 of each qudit. Violation of the CGLMP inequality ($I > 2$) occurs in a wide range of realistic parameters (thick line).

and $J_{23} = 3 \times 10^{-3}$ meV between neighboring spins, as well as axial zero-field splitting parameters $D_1 = -3 \times 10^{-2}$ meV and $D_3 = -2 \times 10^{-2}$ meV. All these parameters are reasonable for Cr and Yb subunits and the weak exchange can be achieved in Cr-Yb molecules [69]. Such a configuration enables a direct application of the CGLMP inequality [50], which is designed to test the nonclassicality of correlations in high-dimensional systems. The inequality is constructed from a functional of the joint outcome probabilities:

$$\begin{aligned}
 I = & [P(A_1 = B_1) + P(B_1 = A_2 + 1) + P(A_2 = B_2) \\
 & + P(A_1 = B_2)] - [P(A_1 = B_1 - 1) + P(A_1 = B_2) \\
 & + P(A_2 = B_2 - 1) + P(B_2 = A_1 - 1)] \\
 & + \frac{1}{3} [P(A_1 = B_1 + 1) + P(B_1 = A_2 + 2) \\
 & + P(A_2 = B_2 + 1) + P(B_2 = A_1 + 1)]
 \end{aligned}$$

$$\begin{aligned}
 & - \frac{1}{3} [P(A_1 = B_1 - 2) + P(B_1 = A_2 - 1) \\
 & + P(A_2 = B_2 - 2) + P(B_2 = A_1 - 2)],
 \end{aligned} \quad (11)$$

where $P(X_\alpha = Y_\beta)$ indicates the probability that the outcomes of the local observables X_α and Y_β coincide. In our notation, A_1 and A_2 denote the outcomes of two measurements performed on the first subsystem, and B_1, B_2 those on the second subsystem. The evaluation of the functional I is analogous to that of the Bell operator $\hat{O}_{\text{Bell}}^{(\max)}$ discussed above, and violations of local hidden-variable models are observed for $I > 2$.

To test the CGLMP inequality with maximal violation, we target the maximally entangled state

$$|\psi\rangle = \frac{1}{\sqrt{4}} \sum_{m=0}^3 |m\rangle_A \otimes |m\rangle_B, \quad (12)$$

and prior to measurements we apply four unitary transformations $U_i^{(A)}$ and $U_j^{(B)}$ ($i, j = 1, 2$) [50,70] with matrix elements

$$[U_i^{(A)}]_{kl} = \frac{1}{\sqrt{4}} e^{\frac{2\pi i l}{4}(\alpha_i + k)}, \quad [U_j^{(B)}]_{kl} = \frac{1}{\sqrt{4}} e^{\frac{2\pi i l}{4}(\beta_j - k)}. \quad (13)$$

Here, $\alpha_1 = 0, \alpha_2 = \frac{1}{2}, \beta_1 = \frac{1}{4},$ and $\beta_2 = -\frac{1}{4}$ [70].

Finally, expectation values of S_z are computed. In the same spirit of the previous section, we test the protocol on the proposed molecular setup by performing numerical simulations of the whole pulse sequence in presence of decoherence. To this goal, we initialize the system in the ground state $|-3/2\rangle_1 \otimes |-1/2\rangle_2 \otimes |-3/2\rangle_3$ and we drive it, through a sequence of single- and two-qudit gates (see the Supplemental Material [56]), to the target state

$$\begin{aligned}
 |\psi\rangle = & \frac{1}{2} \left(\left| -\frac{3}{2}, -\frac{3}{2} \right\rangle + \left| -\frac{1}{2}, -\frac{1}{2} \right\rangle + \left| \frac{1}{2}, \frac{1}{2} \right\rangle \right. \\
 & \left. + \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right)_{13} \otimes \left| -\frac{1}{2} \right\rangle_2,
 \end{aligned} \quad (14)$$

corresponding to a maximally entangled state of the two qudits. The effective interaction between the two qudits is controlled via a central ancilla qubit that acts as a switchable mediator. When the ancilla is frozen in its ground state, no entangling interaction takes place. Conversely, by a conditional excitation of the ancilla depending on the state of both qudits, we implement a two-qudit controlled-phase gate, which turns on qudit-qudit entanglement [10,34,71,72]. After the entangling interaction, the ancilla is returned to its ground state, yielding a final state in which the ancilla qubit is factorized from the two entangled qudits.

The sequence is simulated by solving the Lindblad master equation, exploring realistic pulse amplitudes and dephasing times to identify the optimal trade-off between leakage and decoherence. Remarkably, the much shorter coherence time of the Yb (trensals) ancilla (we use here $T_2 = 1 \mu\text{s}$) has only a limited role, because the ancilla is brought to a superposition only during the implementation of two-qudit gates. Optimized fidelities with the exact state are above 0.91 for each of the considered T_2 values of the qudits (between 5 and 30 μs). In all considered dephasing scenarios, the Bell inequality threshold

of $I = 2$ is clearly exceeded, reaching values up to $I = 2.61$ for $T_2 = 30 \mu\text{s}$, as shown in Fig. 2.

In summary, this work demonstrates the significant potential of molecular nanomagnets as a robust and versatile platform for exploring the quantum properties of matter, particularly within the less-explored territory of multidimensional quantum systems (qudits). In particular, we have shown by numerical simulations based on experimentally measured system parameters and on a feasible experimental setup that ^{173}Yb (trensai) electronuclear spin dimer can be used to probe entanglement by testing generalized Bell inequalities. Moreover, we have proposed an extension of the scheme to a spin-qudit dimer in which the entanglement between the two qudits can be dynamically switched on and off by exciting an interposed qubit switch. These results place molecular nanomagnets as strong candidates not only for applicative issues but also for understanding fundamental quantum phenomena such as qudit-qudit entanglement.

An interesting evolution of the present study involves the derivation and test of inequalities for the qubit-qudit case beyond the CHSH ones, in particular based on nondichotomic measurements.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [83].

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