Nonlocality and entanglement in the XY model

J. Batle* and M. Casas

Departament de Física and Instituto de Física Interdisciplinar y Sistemas Complejos—Consejo Superior de Investigaciones Científicas (IFISC–CSIC), Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain

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Nonlocality and quantum entanglement constitute two special features of quantum systems of paramount importance in quantum-information theory (QIT). Essentially regarded as identical or equivalent for many years, they constitute different concepts. Describing nonlocality by means of the maximal violation of two Bell inequalities, we study both entanglement and nonlocality for two and three spins in the XY model. Our results shed light on the description of nonlocality and the possible information-theoretic task limitations of entanglement in an infinite quantum system.

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I. INTRODUCTION

Schrödinger's contribution [1] to the solution of the paradox posed by Einstein, Podolsky, and Rosen (EPR) [2] motivated the modern notion of entanglement in a quantum system. EPR suggested a description of nature, called “local realism,” which assigned independent properties to distant parties of a composite physical system, to conclude that quantum mechanics (QM) was an incomplete theory. Schrödinger, in turn, regarded entanglement as *the* characteristic feature of QM.

The most significant progress toward the resolution of the EPR debate was made by Bell [3]. Bell showed that local realism, in the form of local variable models (LVMs), implied constraints on the predictions of spin correlations, known as Bell inequalities. Spatially separated observers share an entangled state, and performing measurements on them may induce (nonlocal) correlations that cannot be simulated by local means (they violate Bell inequalities). This limitation to our physical understanding is nowadays exploited for implementing information-theoretic tasks.

Ever since Bell's contribution, entanglement and nonlocality were essentially identified as the same thing. With the advent of quantum-information theory (QIT), interest in entanglement dramatically increased over the years because it lies at the basis of several important processes and applications that possess no classical counterpart [4,5].

Confusion between nonlocality and entanglement arose when the usefulness of quantum correlations was doubted (see Ref. [6]). The nonlocal character of entangled states was clear for pure states because all entangled pure states of two qubits violate the Clauser-Horne-Shimony-Holt (CHSH) inequality and are therefore nonlocal (Gisin's theorem) [7]. However, the situation became more involved when Werner [8] discovered that while entanglement is necessary for a state to be nonlocal, for mixed states is not sufficient. Indeed, an entangled state does not necessarily violate a Bell-type inequality. If not, we say that it admits a local variable model. Werner [8] provided a family of mixed states that does not violate the aforementioned inequalities. Werner also stated

the current mathematical separability definition: A state of a composite quantum system (two subsystems A and B) is called “entangled” if it cannot be represented as a convex linear combination of product states. In other words, the density matrix $\rho_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$ represents an entangled state if it cannot be expressed as

$$\rho_{AB} = \sum_k p_k \rho_A^{(k)} \otimes \rho_B^{(k)}, \quad (1)$$

with $0 \leq p_k \leq 1$ and $\sum_k p_k = 1$. On the contrary, states of the form (1) are called separable. The above definition is physically meaningful because entangled states (unlike separable states) cannot be prepared locally by acting on each subsystem individually [9].

Entanglement is commonly viewed as a useful resource for various information-processing tasks. Yet there exist certain procedures, such as device-independent quantum key distribution [10] and quantum communication complexity problems [11], which can only be carried out provided the corresponding entangled states exhibit nonlocal correlations. Therefore, we are naturally led to the question of whether nonlocality and entanglement constitute two different resources. Throughout the article, and in order to avoid confusion, we will refer to the quantity “nonlocality” as the “maximum violation of a Bell inequality.” The usual meaning of nonlocality (or that of a nonlocal state) as a concept involving the mere violation of a Bell inequality remains the same.

The purpose of the present work is to shed some light upon the relation between entanglement and nonlocality, through the maximal violation of a Bell inequality, in an infinite system, namely, the XY model [12].

The model Hamiltonian of the anisotropic one-dimensional spin- $\frac{1}{2}$ XY model in a transverse magnetic field h for N particles is given by

$$H = \sum_{j=1}^N [(1 + \gamma) S_x^j S_x^{j+1} + (1 - \gamma) S_y^j S_y^{j+1}] - h \sum_{j=1}^N S_z^j, \quad (2)$$

where $\sigma_u^j = 2S_u^j$ ($u = x, y, z$) are the Pauli spin- $\frac{1}{2}$ operators on site j , $\gamma \in [0, 1]$, and $\sigma_u^{j+N} = \sigma_u^j$. The XY model (2) for $N = \infty$ is completely solved by applying a Jordan-Wigner transformation [12,13], which maps the Pauli (spin- $\frac{1}{2}$)

*vdfsjbv4@uib.es

algebra into canonical (spinless) fermions. This model (except for the isotropic case $\gamma = 0$) undergoes a paramagnetic-to-ferromagnetic quantum-phase transition (QPT) [14] driven by the parameter h at $h_c = 1$ and $T = 0$. A QPT is a qualitative change that occurs in the ground state of a many-body system owing to modifications either in the interactions among its constituents or with an external probe.

We will provide evidence for an anomaly that regards entanglement and nonlocality in the XY model. To such an end, we will consider the correlations existing between two sites or qubits (bipartite case) in Sec. II and three sites or qubits (tripartite case) in Sec. III. Finally, some conclusions are drawn in Sec. IV.

II. TWO QUBITS

The general two-site density matrix is expressed as

$$\rho_{ij}^{(R)} = \frac{1}{4} \left(\mathbb{I} + \sum_{u,v} T_{uv}^{(R)} \sigma_u^i \otimes \sigma_v^j \right). \quad (3)$$

$R = j - i$ indicates the distance between spins, $\{u, v\}$ denotes any index of $\{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}$, and $T_{uv}^{(R)} \equiv \langle \sigma_u^i \otimes \sigma_v^j \rangle$. Owing to symmetry considerations, only $\{T_{xx}^{(R)}, T_{yy}^{(R)}, T_{zz}^{(R)}, T_{xy}^{(R)}\}$ do not vanish. Barouch *et al.* [13] provided exact expressions for two-point correlations, together with all the dynamics associated with an external $h(t)$. Let us consider the case where h jumps from an initial value h_0 to a final value h_f at $t = 0$ (the equilibrium case is easily recovered when $h_f = h_0$) and the $R = 1$ configuration. Following Ref. [13], one obtains $T_{xx}^{(1)} = G_{-1}$, $T_{yy}^{(1)} = G_1$, $T_{zz}^{(1)} = G_0^2 - G_1 G_{-1} - S_1 S_{-1}$, and $T_{xy}^{(1)} = S_1$, where

$$\begin{aligned} G_R &= \frac{\gamma}{\pi} \int_0^\pi d\phi \sin(R\phi) \frac{\tanh[\frac{1}{2}\beta\Lambda(h_0)]}{\Lambda(h_0)\Lambda^2(h_f)} \\ &\quad \times [\gamma^2 \sin^2 \phi + (h_0 - \cos \phi)(h_f - \cos \phi) \\ &\quad - (h_0 - h_f)(h_f - \cos \phi) \cos(2\Lambda(h_f)t)] \\ &\quad - \frac{1}{\pi} \int_0^\pi d\phi \cos(R\phi) \frac{\tanh[\frac{1}{2}\beta\Lambda(h_0)]}{\Lambda(h_0)\Lambda^2(h_f)} \\ &\quad \times \{[\gamma^2 \sin^2 \phi + (h_0 - \cos \phi)(h_f - \cos \phi)] \\ &\quad \times (\cos \phi - h_f) - (h_0 - h_f)\gamma^2 \sin^2 \phi \cos \\ &\quad \times [2\Lambda(h_f)t]\}, \end{aligned} \quad (4)$$

$$S_R = \frac{\gamma(h_0 - h_f)}{\pi} \int_0^\pi d\phi \sin(R\phi) \sin \phi \frac{\sin[2\Lambda(h_f)t]}{\Lambda(h_0)\Lambda(h_f)}, \quad (5)$$

with $\Lambda(h) = [\gamma^2 \sin^2 \phi + (h - \cos \phi)^2]^{1/2}$. G_R is the two-point correlator appearing in the Wick theorem calculations, and $M_z = \frac{1}{2}G_0$.

Most of our knowledge on Bell inequalities and their quantum-mechanical violation is based on the CHSH inequality [7]. With two dichotomic observables per party, it is the simplest nontrivial Bell inequality for the bipartite case with binary inputs and outcomes. Quantum mechanically, these observables reduce to $\mathbf{A}_j(\mathbf{B}_j) = \mathbf{a}_j(\mathbf{b}_j) \cdot \boldsymbol{\sigma}$, where $\mathbf{a}_j(\mathbf{b}_j)$ are

unit vectors in $\mathbb{R}^3$ and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. Violation of CHSH inequality requires $\text{Tr}(\rho_{ij}^{(R)} B_{\text{CHSH}})$, that is, the expectation value of the operator B_{CHSH} ,

$$\mathbf{A}_1 \otimes \mathbf{B}_1 + \mathbf{A}_1 \otimes \mathbf{B}_2 + \mathbf{A}_2 \otimes \mathbf{B}_1 - \mathbf{A}_2 \otimes \mathbf{B}_2, \quad (6)$$

is greater than 2. We shall take the optimum value over all $\{\mathbf{a}_j, \mathbf{b}_j\}$ as a proper measure for nonlocality for our state $\rho_{ij}^{(R)}$ [Eq. (3)]. Although this procedure is presented extensively elsewhere [15], we shall provide some details of the calculations here. Given a general two-qubit state ρ in the usual computational basis, we change it into the well-known Bell basis $\{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle\}$. We do so in order to have a physically motivated basis to work with, besides the fact that the concomitant optimization procedure becomes considerably more simple. The ensuing matrix $\rho = \rho_{\parallel} + \rho_{\perp}$ is then decomposed into two contributions, where only terms in $\rho_{\parallel}$,

$$\begin{pmatrix} \rho_{11} & i\rho_{12}^I & i\rho_{13}^I & \rho_{14}^R \\ -i\rho_{12}^I & \rho_{22} & \rho_{23}^R & i\rho_{24}^I \\ -i\rho_{13}^I & \rho_{23}^R & \rho_{33} & i\rho_{34}^I \\ \rho_{14}^R & -i\rho_{24}^I & -i\rho_{34}^I & \rho_{44} \end{pmatrix}, \quad (7)$$

contribute to $\text{Tr}(\rho B_{\text{CHSH}})$, as one can easily check. That is, $\text{Tr}(\rho B_{\text{CHSH}}) = \text{Tr}(\rho_{\parallel} B_{\text{CHSH}}) + \text{Tr}(\rho_{\perp} B_{\text{CHSH}}) = \text{Tr}(\rho_{\parallel} B_{\text{CHSH}})$. The superscripts of the matrix elements in Eq. (7) refer to the concomitant real (R) and imaginary (I) parts. In the XY model, state (3) is almost Bell diagonal except for $\rho_{12}^I = \frac{1}{2}T_{xy}^{(R)}$, which is null in equilibrium ($h_f = h_0$).

The optimization procedure is carried out in two steps: (i) We first parametrize the observers' settings $\{\mathbf{a}_j, \mathbf{b}_j\}$ in spherical coordinates (recall that they are unit vectors in $\mathbb{R}^3$), and then (ii) we obtain, after some algebra, the corresponding optimum value of $\text{Tr}(\rho B_{\text{CHSH}})$ for a specific configuration of the $\{\mathbf{a}_j, \mathbf{b}_j\}$ values. Generically, the final output is $2\sqrt{2}\sqrt{(\rho_{11} - \rho_{44})^2 + (\rho_{22} - \rho_{33})^2 + 4(\rho_{12}^I)^2}$, with the diagonal elements of Eq. (7) arranged so that $\rho_{11} > \rho_{22} > \rho_{33} > \rho_{44}$. The particular form for our state (3) reads as

$$\begin{aligned} B_{\text{CHSH}}^{\max} &\equiv \max_{\mathbf{a}_j, \mathbf{b}_j} \text{Tr}(\rho_{ij}^{(R)} B_{\text{CHSH}}) \\ &= 2\sqrt{\|\mathbf{T}^{(R)}\|^2 - \min_{xyz} + 2[T_{xy}^{(R)}]^2}, \end{aligned} \quad (8)$$

where $\mathbf{T}^{(R)} = (T_{xx}^{(R)}, T_{yy}^{(R)}, T_{zz}^{(R)})$ and $\min_{xyz} \equiv \min([T_{xx}^{(R)}]^2, [T_{yy}^{(R)}]^2, [T_{zz}^{(R)}]^2)$. This functional form for the optimum value $B_{\text{CHSH}}^{\max}$ is reminiscent of the aforementioned arrangement of the diagonal elements of Eq. (7) in our case (3). Figure 1 depicts the evolution of nonlocality (8) for the case $\gamma = 0.5$ and ($h_0 = 0.5, h_f = 0$). For $\gamma = 1$ (Ising) and ($h_0 = h_c, h_f = 0$), Eq. (8) would oscillate indefinitely. This nonlocality measure oscillates around a value distinct from the one expected. Just as in the case of M_z in Ref. [13], or entanglement in the XY model [16] (as measured by the concurrence C), Eq. (8) does not reach its equilibrium value, which entails that nonlocality is also a nonergodic quantity. The introduction of the nonergodicity issue in the present context for our nonlocality measure [Eq. (8)] is justified because our aim is to pursue all those

FIG. 1. (Color online) The oscillating curve depicts $B_{\text{CHSH}}^{\text{max}}$ [Eq. (8)] vs time (in s) for $h_0 = 0.5, h_f = 0, \gamma = 0.5$, and $R = 1$ for the evolved state $\rho_{ij}^{(R)}(t)$ [Eq. (3)] at $T = 0$. Final and equilibrium values do not coincide (*nonergodic*). Inset (a) depicts $B_{\text{CHSH}}^{\text{max}}$ vs h for $\gamma = 0.5$ and different distances between spins $R = 1, 2, 3$, and ∞ (dotted line). Though no Bell violation is observed, $B_{\text{CHSH}}^{\text{max}}$ exhibits a long-range order. Inset (b) depicts equilibrium nonlocality (upper curves) and concurrence (lower curves) measures vs h for $\gamma \in [0, 1]$ and $R = 1$. The isotropic case $\gamma = 0$ collapses to 2 for $h \geq 1$. See the text for details.

aspects that are common to both entanglement and nonlocality. Because it is known that quantum entanglement displays such a feature for the bipartite case in the XY model [16], we show that this behavior is a characteristic aspect of nonlocality as well, which is a physical resource intimately related to entanglement. In fact, both entanglement and nonlocality are mathematically expressed in terms of the two-point correlation functions in Eq. (3), which in turn are nonergodic quantities after the action of some quench, as first pointed out by Barouch *et al.* in Ref. [13].

The equilibrium case ($h_f = h_0$) is considered in Fig. 1(a). $B_{\text{CHSH}}^{\text{max}}$ evolves for several configurations, namely, $R = 1$ (upper solid curve), $R = 2$ (middle solid curve), $R = 3$ (lower solid curve), and $R = \infty$ (dotted line) [13]. It is apparent that nonlocality exhibits a long-range behavior, while C rapidly tends to zero [17]. A comparison with entanglement appears in Fig. 1(b) for $R = 1$ and γ anisotropies ranging from 0 to 1 at intervals of 0.1. As the amount of anisotropy increases, nonlocality displays an overall increasing (decreasing) tendency before (after) the QPT at $h_c = 1$, while entanglement C goes in the opposite direction. The usefulness of (bi)entanglement between spins in the XY model is questioned in quantum-information processing by the fact that the concomitant correlations never violate a Bell inequality ($B_{\text{CHSH}}^{\text{max}} \leq 2 \forall h, \gamma$).

All previous quantities are ultimately described in terms of several G_R , so that they all diverge at $h = 1$ in the same manner. Let us consider for simplicity $M_z(h) = \frac{1}{2}G_0 = \frac{\partial}{\partial h} \frac{1}{2\pi} \int_0^\pi d\phi [\gamma^2 \sin^2 \phi + (h - \cos \phi)^2]^{1/2}$. For $\gamma = 1$, we have $M_z(h) = \frac{\partial}{\partial h} [\frac{2(h+1)}{2\pi} E(\frac{2\sqrt{h}}{h+1})] = \frac{1}{2\pi} [\frac{h-1}{h} K(\frac{2\sqrt{h}}{h+1}) + \frac{h+1}{h} E(\frac{2\sqrt{h}}{h+1})]$, where $K(E)$ is the complete elliptic integral of the first (second) kind. Then $\frac{d}{dh} M_z$ diverges logarithmically

at $h = 1$, following the divergence of K , and so does (the first derivative of) C and $B_{\text{CHSH}}^{\text{max}}$, including nonequilibrium ($t = \infty$) values. Therefore, entanglement and nonlocality exhibit one additional feature beside nonergodicity: They both signal the presence of a QPT at $T = 0$.

III. THREE QUBITS

Nonlocality in the three-qubit case is explored through the violation of the Mermin inequality [18]. The Mermin inequality reads as $\text{Tr}(\rho B_{\text{Mermin}}) \leq 2$, where B_{Mermin} is the Mermin operator,

$$B_{\text{Mermin}} = B_{a_1 a_2 a_3} - B_{a_1 b_2 b_3} - B_{b_1 a_2 b_3} - B_{b_1 b_2 a_3}, \quad (9)$$

with $B_{uvw} \equiv \mathbf{u} \cdot \boldsymbol{\sigma} \otimes \mathbf{v} \cdot \boldsymbol{\sigma} \otimes \mathbf{w} \cdot \boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the usual Pauli matrices and $\mathbf{a}_j$ and $\mathbf{b}_j$ are unit vectors in $\mathbb{R}^3$. Notice that Greenberger-Horne-Zeilinger (GHZ) states maximally violate the Mermin inequality. As usual, we will employ

$$\mathcal{M}^{\text{max}} \equiv \max_{\mathbf{a}_j, \mathbf{b}_j} \text{Tr}(\rho B_{\text{Mermin}}) \quad (10)$$

as a measure for the nonlocality of the state ρ . Obviously, the Mermin inequality is not the only existing Bell inequality for three qubits, but because it constitutes a simple generalization of the CHSH to the tripartite case, it will be enough to make use of this particular inequality to illustrate the basic results of the present work.

The XY model is completely solvable, a fact that allows us to compute—as in the previous case of two sites—the reduced density matrix for three spins without the explicit construction of the global infinite state of the system. The reduced state of three spins reads as

$$\rho_{ijk}^{(a,b)} = \frac{1}{8} \left(\mathbb{I} + \sum_{u,v,w} T_{uvw}^{(a,b)} \sigma_u^i \otimes \sigma_v^j \otimes \sigma_w^k \right), \quad (11)$$

where $i < j < k$ indicates the positions of the three spins, $a = j - i, b = k - j$ indicate their relative distances. $\{u, v, w\}$ denotes indexes of the Pauli matrices $\{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}$, and $T_{uvw}^{(a,b)} \equiv \langle \sigma_u^i \otimes \sigma_v^j \otimes \sigma_w^k \rangle_{ab}$. Similar to the calculation of the two-spin correlations computed by Barouch *et al.* [13], based in turn on the work by Lieb *et al.* [12], we extend them to the three-party case by using the well-known Wick theorem in quantum-field theory. Owing to the symmetry of the XY model, some of them vanish. Furthermore, as far as nonlocality is concerned, among those correlations that survive, only four of them contribute to Eq. (10), namely, $T_{xxz}^{(a,b)}, T_{xzx}^{(a,b)}, T_{zxx}^{(a,b)}$, and $T_{zzz}^{(a,b)}$. These three-spin correlation functions $T_{xxz}^{(a,b)}, T_{xzx}^{(a,b)}$, and $T_{zzz}^{(a,b)}$ are given by

$$\begin{vmatrix} G_{-1} & \dots & G_{-a+1} & G_{-a-1} & \dots & G_{-a-b} \\ \vdots & & \vdots & \vdots & & \vdots \\ G_{a-2} & \dots & G_0 & G_{-2} & \dots & G_{-b-1} \\ G_a & \dots & G_2 & G_0 & \dots & G_{-b+1} \\ \vdots & & \vdots & \vdots & & \vdots \\ G_{a+b-2} & \dots & G_b & G_{b-2} & \dots & G_{-1} \end{vmatrix}, \quad (12)$$

$$\begin{pmatrix} G_{-1} & \dots & G_{-a} & G_{-a-b} \\ G_0 & \dots & G_{-a+1} & G_{-a-b+1} \\ \vdots & \ddots & \vdots & \vdots \\ G_{a-2} & \dots & G_{-1} & G_{-b-1} \\ G_{a+b-1} & \dots & G_b & G_0 \end{pmatrix}, \quad (13)$$

$$\begin{pmatrix} G_0 & G_{-a} & G_{-a-b} \\ G_a & G_0 & G_{-b} \\ G_{a+b} & G_b & G_0 \end{pmatrix},$$

respectively, with $T_{zxx}^{(a,b)} = T_{xxz}^{(b,a)}$ owing to translational symmetry.

Correlations between parties strongly depend on their relative positions a and b . We shall distinguish two types: (i) The one forming a block of three in consecutive sites ($a = b = 1$), as well as a centered configuration ($a = b = 2$), and (ii) two nearest-neighbor spins plus an additional one ($a = 1, b = 2$).

Optimization of $\mathcal{M}^{\max}$ [Eq. (10)] for any configuration of the spins along the chain is carried out in the same fashion as in the previous bipartite case. Once the observers' settings $\{\mathbf{a}_j, \mathbf{b}_j\}$ are parametrized in spherical coordinates $(\sin \theta_k \cos \phi_k, \sin \theta_k \sin \phi_k, \cos \theta_k)$, the problem consists in finding the supremum of Eq. (10) over the set of $\{k = 1 \dots 12\}$ possible angles. Here, too, we will consider ground-state nonlocality.

Let us consider the block configuration $a = b = 1$. The orientation of the settings $\{\mathbf{a}_j, \mathbf{b}_j\}$ that maximizes $\mathcal{M}^{\max}$ [Eq. (10)] is such that (x - z plane only, that is, we deal with *real qubits* for $u_j^y = 0 \ \forall \mathbf{u}$) $\{\mathbf{a}_3 = -\mathbf{a}_1, \mathbf{b}_1 = \mathbf{a}_2, \mathbf{b}_2 = -\mathbf{a}_1, \mathbf{b}_3 = -\mathbf{a}_2\}$ for the whole range of h . Explicitly, $\mathcal{M}^{\max} = \max_{\theta_{a_1}, \theta_{a_2}} (a_2^z [(a_2^z)^2 - 3(a_1^z)^2] T_{zzz}^{(1,1)} + \{a_2^z [(a_2^x)^2 - (a_1^x)^2] - 2a_1^z a_2^x (T_{zxx}^{(1,1)} + T_{xxz}^{(1,1)} + T_{xxz}^{(1,1)})\})$. The ensuing analytic form of $\mathcal{M}^{\max}$ vs h —a complicated rational function with radicals—is calculated by recourse to convex optimization. For the sake of generality, let us also consider the centered configuration $a = b = 2$. After some algebra, we obtain that one disposition of the observers that provides an analytical expression for a lower bound to Eq. (10) is given by (again in the x - z plane) $\{\mathbf{a}_1 = (\sin \theta_{a_1}, \cos \theta_{a_1}), \mathbf{a}_2 = (0, -1), \mathbf{a}_3 = (\sin \theta_{a_1}, -\cos \theta_{a_1}), \mathbf{b}_1 = \mathbf{a}_3, \mathbf{b}_2 = (1, 0), \mathbf{b}_3 = -\mathbf{a}_1\}$. Hence, we obtain $\max_{\theta_{a_1}} (2 \cos^2 \theta_{a_1} T_{zzz}^{(2,2)} + 2 \sin \theta_{a_1} \cos \theta_{a_1} T_{zxx}^{(2,2)} - 2 \sin^2 \theta_{a_1} T_{xxz}^{(2,2)} + 2 \sin \theta_{a_1} \cos \theta_{a_1} T_{xxz}^{(2,2)}) \leq \mathcal{M}^{\max} \leq \sqrt{4(T_{zzz}^{(2,2)})^2 + 4(T_{zxx}^{(2,2)})^2 + 4(T_{xxz}^{(2,2)})^2 + 4(T_{xxz}^{(2,2)})^2}$. The analytic form of the lower bound (not provided here) is of the same nature as that of the $a = b = 1$ case. In fact, the lower bound becomes an equality for all (a, b) shortly before $h = 1$. Additionally, the upper bound also applies to all configurations.

Figures 2(a) and 2(b) present the situation where $\mathcal{M}^{\max}$ is depicted for different values of the γ anisotropy and different configurations of the spins. Numerical calculations agree perfectly with the corresponding analytic expressions. As h grows, the state $\rho_{ijk}^{(a,b)}$ approaches $|\downarrow\downarrow\downarrow\rangle\langle\downarrow\downarrow\downarrow|$ as expected (ferromagnetic phase), and *never violates the Mermin inequality*, which entails an inherent limitation to the usefulness of entanglement itself.

FIG. 2. (Color online) (a) Value of $\mathcal{M}^{\max}$ vs h (10) for several γ values for the $a = b = 1$ block configuration. (b) Similar curves for $a = 1, b = 2$ and $a = 2, b = 2$, with $\gamma = 0.5$. (c) Evolution of multipartite entanglement S_{vN} ($a = b = 1$) vs h for several values of the anisotropy. (d) $\mathcal{M}^{\max}$ vs S_{vN} plots for $\gamma = 0.5$ and all previous configurations, $a = b = 1$, $a = 1, b = 2$, and $a = b = 2$. Notice the apparent monotonic decreasing evolution. See the text for details.

Characterization of entanglement is of paramount relevance in QIT [19], yet, as far as we know, no operational measure is available to date that quantifies genuine multipartite entanglement. However, some measures (for pure states) based on partitions of the system have been advanced, such as the so-called “global entanglement” (GE), which describes the average entanglement of each qubit of the system with the remaining $(N - 1)$ qubits. The GE measure is widely regarded as a legitimate, useful, and practical N -qubit entanglement measure [20–22]. Our state $\rho_{ijk}^{(a,b)}$ [Eq. (11)] of three spins is, in general, mixed, which implies that the previous measures do not apply as such.

The extension of these partition-based entanglement measures to the case of mixed states is formally performed by recourse to the usual convex roof [4] defined over some given set of pure states. Because we would require an extraordinary numerical effort to operationally employ such measure, we will nevertheless make use of the sum of the von Neumann entropy of the reduced density matrices of the three spins of $\rho_{ijk}^{(a,b)}$, $S_{vN} = 3S_{vN}(\rho_i)$, with $\rho_i = \frac{1}{2}(\mathbb{I} + \langle \sigma_z \rangle \sigma_z^i)$, $\langle \sigma_z \rangle = G_0 = 2M_z$. This measure might not grasp, for instance, all the exact details of the ongoing QPT, but it nevertheless constitutes a physically motivated quantity and is a simple tool with which to compare nonlocality, where no definition problem arises regardless of the number of parties involved. Incidentally, it has also been considered as a proper entanglement measure in the literature [23].

We shall consider ground-state entanglement ($T = 0$) as well. The specific form of S_{vN} is depicted in Fig. 2(c) for several values of the γ anisotropy as a function of h . The monotonic decreasing tendency of entanglement is apparent for any γ value. As h grows, the fidelity between $\rho_{ijk}^{(a,b)}$ and the final state (the one corresponding to $h = \infty$) steadily tends to 1. Remarkably, we observe opposite tendencies revealed by entanglement S_{vN} and nonlocality [Eq. (10)]. Recall that our

model undergoes a second-order QPT in the ground energy. In fact, because $\frac{d}{dh} S_{vN} \propto \frac{d}{dh} M_z$, this measure of multipartite entanglement (its derivative) diverges logarithmically at $h_c = 1$. Also, notice that a proper GE extension of the S_{vN} measure for mixed states would also diverge in the same fashion owing to the linearity of the convex hull procedure. For other entanglement measures that take into account the symmetry broken in the QPT of Hamiltonian (2), see Refs. [23] and [24]. Surprisingly, our measure of nonlocality [Eq. (10)] also displays such a divergence, along with its bounds. In Fig. 2(d) we show the dependency of $\mathcal{M}^{\max}$ versus entanglement S_{vN} for several values of γ in the $(a = 1, b = 1)$ configuration. Finally, we encounter a multipartite system where both entanglement (its first derivative) and nonlocality are good indicators of a QPT.

IV. CONCLUSIONS

We have studied how nonlocality—measured by the maximal violation of a Bell inequality—compares to entanglement

in a condensed matter system. Although two instances (two and three sites) have been considered, our results may properly generalize to any block of spins. For the bipartite case, we have computed the exact value of $B_{\text{CHSM}}^{\max}$ during time evolution and in equilibrium. In either case our nonlocality measure [Eq. (8)] displays a nonergodic behavior, it is able to detect a QPT, and limits the QIT-related tasks involving bipartite entanglement along the infinite chain because no Bell inequality is violated. A similar situation occurs in the tripartite case, where nonviolation of local realism in the XY model takes place as well. Also, entanglement and nonlocality both indicate a QPT yet they exhibit opposite evolutions in the phase diagram. Finally, nonlocality can also constitute a complementary resource in infinite quantum systems.

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