Characterization of quantum phase transition in the XY model with multipartite correlations and Bell-type inequalities

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The ground state of interacting spin chains in external magnetic fields can undergo a quantum phase transition (QPT) characterized by dramatic changes at a critical value of the magnetic field. In this paper, we use Bell-type inequalities to study the multipartite correlations (including multipartite entanglement and multipartite nonlocality in an n-spin subsystem) in the QPT of an infinite XY chain. An efficient numerical optimization procedure is proposed to figure out the violation measure M_n of the inequalities. For $n \leqslant 7$, the magnetic-field (λ) dependence of M_n is studied. We find the derivative of M_n is divergent exactly at the QPT point $\lambda_c = 1$ for any n. In addition, with the increase of n, M_n converges quickly for $\lambda < \lambda_c$ and converges very slowly for $\lambda > \lambda_c$, which can be regarded as another signal for the QPT. Furthermore, in the vicinity of λ_c, high-order Bell-type inequalities will be violated as long as n is large enough. This indicates that high-level multipartite correlation will be present when the system is in the vicinity of the QPT point. Nevertheless, genuine n-partite entanglement or genuine n-partite nonlocality is not observed in the QPT.

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I. INTRODUCTION

Quantum entanglement is one of the most important concepts in quantum mechanics and quantum information theory [1]. In the field of condensed-matter physics, quantum entanglement has attracted much attention, partly because it provides interesting perspectives for us to understand quantum phase transitions (QPTs) [2]. A QPT is the dramatic change of the ground state of a macroscopic quantum system. Bipartite measures of entanglement, such as the entanglement concurrence and the entanglement entropy, have been found to show a maximum, a singularity, or an interesting logarithmic scaling behavior in the vicinity of the QPT points [3–10]. These findings greatly enhance our understanding of QPTs.

Another way to characterize the correlations at a QPT is to investigate the quantum nonlocality. Nonlocality is also a kind of quantum correlation, which is indicated by the violation of Bell-type inequalities [11–13]. It is a natural conjecture that nonlocality should also play a fundamental role in QPTs, just as entanglement does. However, it is rather surprising that bipartite nonlocality is not observed in most one-dimensional models [14–18]. Recently, it was pointed out by Oliveira *et al.* that the absence of bipartite nonlocality in translationally invariant systems results from the monogamy inequality obeyed by quantum nonlocality [19]. As a result, the basic role of quantum nonlocality in QPTs of one-dimensional spin models remains unclear.

With the help of the Mermin inequality and the Svetlichny inequality, recently, Bell-type inequalities have been generalized to multipartite settings, which makes them natural candidates for a quantitative evaluation of quantum nonlocality in any multipartite setting [20–26]. For example, Batle and Casas have investigated the nonlocality in subsystems with three qubits ($n = 3$) in infinite XY chains [27]. Unfortunately, for various choices of three spins, nonlocal correlation is not observed. For a quantum Ising model with finite spins (up to seven spins), the nonlocality has been studied [28]. However, as the length of the system is too small, the relationship between multipartite nonlocality and QPT has not been discussed.

In this paper we will use generalized Bell-type inequalities to characterize the multipartite correlation in the QPT of infinite XY chains. First, we propose an efficient procedure to calculate the violation measure of the inequalities, which greatly reduces the CPU time in numerical optimization. Second, we find that high-order inequalities are just violated in the vicinity of the QPT point, which provides an alternative perspective to understand the link between quantum correlation and QPTs in one-dimensional systems. We would like to mention that the global entanglement of the XY chain has been studied [23,29]. However, as we will show, Bell-type inequalities are defined naturally in multipartite settings. Furthermore, they provide us a unified view of both multipartite entanglement and multipartite nonlocality.

This paper is organized as follows. In Sec. II, we briefly review the concepts of the Mermin inequality and Mermin-Svetlichny inequality. Some technique details about the numerical optimization will also be proposed. In Sec. III, we apply the theory to n continuous spins in infinite XY models. A summary is given in Sec. IV.

II. DEFINITION AND OPTIMIZATION OF n-PARTITE CORRELATIONS

A. n-partite Mermin inequality

In this paper, the main tool to study multipartite correlation is a class of Bell inequalities derived by Mermin, Ardehali, Belinskii, and Klyshko [30–32]. Let's consider an experiment on n parties, where each party performs one out of two measurements. We denote the two outcomes from party j as a_j and a'_j. Letting $M_1 = a_1$ and $M'_1 = a'_1$, the Mermin-Klyshko (MK) polynomials can be defined recursively as

$$M_n = \tfrac{1}{2}M_{n-1}(a_n + a'_n) + \tfrac{1}{2}M'_{n-1}(a_n - a'_n),$$
$$M'_n = \tfrac{1}{2}M'_{n-1}(a'_n + a_n) + \tfrac{1}{2}M_{n-1}(a'_n - a_n),$$

where M_n and M'_n can be obtained from each other by exchanging all the a_j and a'_j. For a given quantum-state described by a density matrix $\hat{\rho}_n$, the polynomial M_n should be interpreted as the expectation value of the corresponding Mermin operator $\hat{M}_n$ [24]. As we will show, $\hat{M}_n$ depends upon $2n$ unit vectors.

Let's take the $n = 2$ case as an example. Now the MK polynomial is expressed as

$$M_2 = \tfrac{1}{2}a_1(a_2 + a'_2) + \tfrac{1}{2}a'_1(a_2 - a'_2).$$

In the context of quantum mechanics, M_2 should be interpreted as the expectation value of $\hat{M}_2$, i.e., $M_2 = \mathrm{Tr}(\hat{\rho}_2\hat{M}_2)$, with

$$\hat{M}_2 = \tfrac{1}{2}\boldsymbol{a_1}\cdot\boldsymbol{\sigma}_1 \otimes (\boldsymbol{a_2} + \boldsymbol{a'_2})\cdot\boldsymbol{\sigma}_2 + \tfrac{1}{2}\boldsymbol{a}\cdot\boldsymbol{\sigma}_1 \otimes (\boldsymbol{a_2} - \boldsymbol{a'_2})\cdot\boldsymbol{\sigma}_2,$$

where $\boldsymbol{a_j}$ and $\boldsymbol{a'_j}$ are unit vectors in R^3 space and $\boldsymbol{\sigma} = (\hat{\sigma}_x,\hat{\sigma}_y,\hat{\sigma}_z)$ are Pauli matrices. One can see that $\hat{M}_2$ is just the widely used Clauser-Horne-Shimony-Holt operator [12], with the two differing by a constant factor.

For any n-partite state $\hat{\rho}_n$ which admits a local hidden-variable theory, it should hold that [24]

$$\mathrm{Tr}(\hat{\rho}_n\hat{M}_n) \leqslant 1. \quad (1)$$

The violation of the above inequality indicates that $\hat{\rho}_n$ cannot be described by any local variable theory; in other words, it contains nonlocal correlation. In this paper we will call $M_n = \mathrm{Tr}(\hat{\rho}_n\hat{M}_n)$ the violation measure of the Mermin inequality. In addition, it has been shown that the inequality will also be violated if $\hat{\rho}_n$ is entangled [24]. Thus, the inequality can be used to indicate both the nonlocality and the entanglement. Suppose a state $\hat{\rho}_n$ violates the above inequality; it would be interesting to further characterize the multipartite nature of the correlations in $\hat{\rho}_n$, discussed in the following.

B. Multipartite entanglement

A two-party state $\hat{\rho}_2$ is separable if it can be decomposed as $\hat{\rho}_2 = \sum_i p_i|\Psi_i\rangle\langle\Psi_i|$, where $|\Psi_i\rangle = |\psi_1\rangle_i|\psi_2\rangle_i$ are product states for all i. In the multipartite case, because of many more choices in decomposing the system, the classification of entanglement is much richer than in the bipartite case [22]. If an n-party state $\hat{\rho}_n$ can be decomposed as $\hat{\rho}_n = \sum_i p_i|\Psi_i\rangle\langle\Psi_i|$, where $|\Psi_i\rangle = |\psi_1\rangle_i\cdots|\psi_n\rangle_i$ are product states for all i, we say $\hat{\rho}_n$ is fully separable. Instead, if any $|\Psi_i\rangle$ can just be expressed as $|\Psi_i\rangle = |\psi_{12}\rangle_i|\psi_3\rangle_i\cdots|\psi_n\rangle_i$, rather than a full product form, we say that $\hat{\rho}_n$ is two-partite entangled. Similarly, one can generalize to the definition of m-partite entanglement. A larger m indicates a higher *hierarchy* of multipartite entanglement.

For an n-partite state containing at most m-partite entanglement ($m \leqslant n$), it should hold that [24]

$$M_n = \mathrm{Tr}(\hat{\rho}_n\hat{M}_n) \leqslant \frac{1}{\sqrt{2}}2^{m/2}. \quad (2)$$

In this paper, we will call it the m-order Mermin inequality. Inequality (1) can be seen as the first-order Mermin inequality. For some state $\hat{\rho}_n$, if the m-order Mermin inequality is violated, there is at least $(m+1)$-partite entanglement in $\hat{\rho}_n$. A state $\hat{\rho}_n$ contains genuine n-partite entanglement if the $(n-1)$-order Mermin inequality is violated. Thus, the violation of Mermin inequalities can be used as a sufficient criterion to classify multipartite entanglement.

C. Multipartite nonlocality

Bancal *et al*. have proposed the so-called grouping models to quantify multipartite nonlocality [26]. Suppose we can divide an n-partite system into m groups, such that within each group the parties can communicate with each other, while between different groups no communication is allowed. We will call it an m-grouping model. It is natural that a smaller m indicates a higher hierarchy of multipartite nonlocality. For example, for $m = n$, the model is fully separable and thus has no nonlocality, while for $m = 1$, the model contains genuine n-partite nonlocality.

First, let's define the Mermin-Svetlichny (MS) operator as

$$\hat{S}_n^m = \begin{cases} \hat{M}_n, & \text{for } n-m \text{ even}, \\ \hat{M}_n^+, & \text{for } n-m \text{ odd}, \end{cases} \quad (3)$$

with $\hat{M}_n^+ = \frac{1}{\sqrt{2}}(\hat{M}_n + \hat{M}'_n)$. Then for any m-grouping model, it holds that [26]

$$S_n^m = \mathrm{Tr}\big(\hat{\rho}_n\hat{S}_n^m\big) \leqslant 2^{(n-m)/2}. \quad (4)$$

In this paper, we will call it the m-order Mermin-Svetlichny inequality for n sites. Inequality (1) can be seen as the n-order Mermin-Svetlichny inequality for n sites. If the m-order Mermin-Svetlichny inequality is violated by a state $\hat{\rho}_n$, in the framework of the grouping models it says that an $m-1$ (or less) grouping model is needed to reproduce the nonlocality in $\hat{\rho}_n$. A state $\hat{\rho}_n$ contains genuine n-partite nonlocality if the second-order Mermin inequality is violated. Thus, the violation of the Mermin-Svetlichny inequality is a sufficient criterion to classify multipartite nonlocality.

D. Details for numerical optimization

As we have shown, M_n (and S_n^m) is a function of the unit vectors $\{\boldsymbol{a_1},\boldsymbol{a'_1},\ldots\}$. For a given $\hat{\rho}_n$, in order to detect the multipartite correlation, one has to find the max value of $\mathrm{Tr}(\hat{\rho}_n\hat{M}_n)$ with respect to $2n$ unit vectors. Multivariable optimization is usually difficult, and large amount of numerical calculation is involved, which may be one of the reasons why the fast-developed quantum information theory about multipartite correlation has not been extensively applied in one-dimensional quantum systems. Thereby, an efficient procedure to carry out the optimization is significant. We would like to mention that an efficient numerical optimization to calculate the global quantum correlation has been proposed in Ref. [33]. In the optimization of M_n, we find that most of the CPU time is used to repeatedly evaluate the value of the objective function $M_n = \mathrm{Tr}(\hat{\rho}_n\hat{M}_n)$ for different sets $\{\boldsymbol{a_1},\boldsymbol{a'_1},\ldots\}$. Now we show how to obtain a high efficiency to evaluate M_n. First, the Mermin operator $\hat{M}_n$ can be expressed as the following inner product:

$$\hat{M}_n = \boldsymbol{f_n} \cdot [\boldsymbol{\sigma}_1 \otimes \cdots \otimes \boldsymbol{\sigma}_n],$$

where $\boldsymbol{f_n}$ is the sum of the dyadic of unit vectors $\{\boldsymbol{a_1}, \boldsymbol{a}'_1, \ldots\}$ and $\boldsymbol{\sigma}_1 \otimes \cdots \otimes \boldsymbol{\sigma}_n$ is regarded as the dyadic of n spin vectors. For example, $\hat{M}_2$ can be rewritten as

$$\hat{M}_2 = \tfrac{1}{2}[\boldsymbol{a_1} \otimes \boldsymbol{a_2} + \boldsymbol{a_1} \otimes \boldsymbol{a}'_2 + \boldsymbol{a} \otimes \boldsymbol{a_2} - \boldsymbol{a} \otimes \boldsymbol{a}'_2] \cdot [\boldsymbol{\sigma}_1 \otimes \boldsymbol{\sigma}_2].$$

Next, we can express the objective function M_n as

$$M_n = \mathrm{Tr}(\hat{\rho}_n \hat{M}_n) = \boldsymbol{f_n} \cdot \boldsymbol{\rho_n}, \tag{5}$$

with

$$\boldsymbol{\rho_n} = \mathrm{Tr}(\hat{\rho}_n[\boldsymbol{\sigma}_1 \otimes \cdots \otimes \boldsymbol{\sigma}_n]).$$

In practice, we treat $\boldsymbol{f_n}$ and $\boldsymbol{\rho_n}$ as vectors. Now all variables of the objective function are contained in vector $\boldsymbol{f_n}$, and all the constants in the objective function are contained in vector $\boldsymbol{\rho_n}$. The optimization of M_n is just to find an optimal vector $\boldsymbol{f_n}$ which has the most amount of overlap with the given vector $\boldsymbol{\rho_n}$. In our program, we figure out the constant vector $\boldsymbol{\rho_n}$ before calling the objective function, rather than evaluating repeatedly the complex matrix-direct-product operations in $\mathrm{Tr}(\hat{\rho}_n \hat{M}_n)$, which greatly improves the efficiency. Furthermore, it should be mentioned that $\boldsymbol{\rho_n}$ is sparse. We find numerically that only about 20% of its elements are nonzero. Consequently, most of the elements in $\boldsymbol{f_n}$ can be omitted, and the objective function $M_n = \boldsymbol{f_n} \cdot \boldsymbol{\rho_n}$ can be dramatically reduced. The separation of variables and constants combined with the reduction of the objective function improves the efficiency of the numerical optimization by about 10 times.

III. MULTIPARTITE CORRELATION IN THE GROUND STATE OF THE *XY* MODEL

A. Solution of the *XY* model

The XY model can be described by the following Hamiltonian:

$$\hat{H} = -\sum_i \left[(1+\gamma)\hat{S}_i^x \hat{S}_{i+1}^x + (1-\gamma)\hat{S}_i^y \hat{S}_{i+1}^y + \lambda \hat{S}_i^z\right],$$

where γ is a dimensionless parameter describing the anisotropy in the x-y plane and λ is a dimensionless parameter characterizing the strength of the magnetic field. The model reduces to the Ising model and XX model for $\gamma = 1$ and $\gamma = 0$, respectively. For $0 < \gamma \leqslant 1$, the ground state of the system undergoes a second-order QPT at the critical point $\lambda_c = 1$. The model is exactly solvable in the thermodynamic limit [34,35]. In this paper, in infinite XY chains with an open boundary condition, we will investigate the multipartite correlation in a subsystem consisting of n consecutive spins, located in the middle of the chain.

The first step is to construct the reduced density matrix of the subsystem, i.e., $\hat{\rho}_n$. According to Barouch *et al.*, $\hat{\rho}_n$ can be expressed in the following (unnormalized) form [34–36]:

$$\hat{\rho}_n = \sum_{\mu_1,\ldots,\mu_n=\{0,x,y,z\}} \langle \hat{S}_1^{\mu_1} \cdots \hat{S}_n^{\mu_n} \rangle \hat{S}_1^{\mu_1} \cdots \hat{S}_n^{\mu_n}, \tag{6}$$

where we have used $\hat{S}_i^0$ to denote the identity matrix. We just need to calculate the n-party correlation functions $\langle \hat{S}_1^{\mu_1} \cdots \hat{S}_n^{\mu_n} \rangle$. First, for any given set of $\{\mu_1, \ldots, \mu_n\}$, we transform $\hat{S}_1^{\mu_1} \cdots \hat{S}_n^{\mu_n}$ into the product of an even number of Majorana operators $\breve{a}_j$ [36]. Then with the help of Wick's theorem from quantum-field theory [37], the average value of the products of $\breve{a}_j$ is expressed in terms of the second moments $\langle \breve{a}_m \breve{a}_n \rangle$. The expressions for $\langle \breve{a}_m \breve{a}_n \rangle$ are well known [36]. Thus, along this procedure, we are able to identify $\hat{\rho}_n$ exactly for finite n. In practice, the symmetry of the model can be utilized; that is, $\langle \hat{S}_1^{\mu_1} \cdots \hat{S}_n^{\mu_n} \rangle$ is equal to zero if the number of μ_i satisfying $\mu_i = x,y$ is odd.

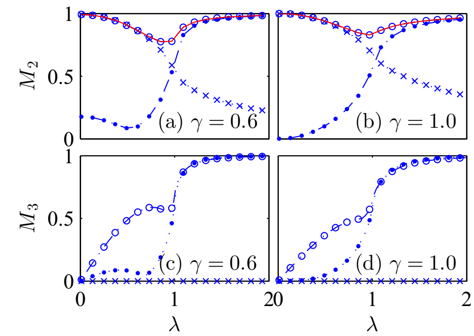

FIG. 1. (Color online) Violation measure M_n ($n = 2,3$) of the Mermin inequality as a function of the dimensionless magnetic-field parameter λ for several values of the dimensionless anisotropic parameter γ. The circles, dots, and crosses are according to M_n with $\{\boldsymbol{a_1}, \boldsymbol{a}'_1, \ldots\}$ in the x-y plane, x-z plane, and y-z plane, respectively. The red lines in (a) and (b) denote the exact results according to Horodecki's formula, divided by 2.

After obtaining $\hat{\rho}_n$, we will use the Mermin inequalities to detect the quantum correlations in $\hat{\rho}_n$. Before starting our study, we have confirmed the validity of our optimization procedure by reproducing some previous results. For $n = 2$, the max value of M_2 can be figured out exactly according to Horodecki *et al.*'s formula [13]. In Figs. 1(a) and 1(b), we show our results for $n = 2$ for several γ. We consider three special situations; that is, all the vectors $\{\boldsymbol{a_1}, \boldsymbol{a}'_1, \ldots\}$ are in the x-y plane, in the x-z plane, or in y-z plane. The exact results according to Horodecki *et al.*'s formula are denoted by red lines. One can see that our numerical results are in good agreement with the exact results. Furthermore, for $n = 3$ [see Figs. 1(c) and 1(d)], the first-order Mermin inequality $\mathrm{Tr}(\hat{\rho}_n \hat{M}_n) \leqslant 1$ is never violated. It means that nonlocality is not observed for three-qubit subsystems, which is consistent with previous results [27].

For $n \geqslant 4$, as we will show, the first-order Mermin inequality is violated when all the vectors $\{\boldsymbol{a_1}, \boldsymbol{a}'_1, \ldots\}$ are in the x-z plane. Thus, in this paper, we will just consider M_n with all $\{\boldsymbol{a_1}, \boldsymbol{a}'_1, \ldots\}$ in the x-z plane.

B. Signals of QPT

For the Ising case ($\gamma = 1$), we show the magnetic-field dependence of M_n and its first-order derivative $\frac{\partial M_n}{\partial \lambda}$ in Fig. 2. First, $\frac{\partial M_n}{\partial \lambda}$ diverges exactly at the critical point $\lambda_c = 1$ for all n [see Fig. 2(b)]. As we have shown in Eq. (6), the elements of $\hat{\rho}_n$ are just multispin correlation functions. They (or part

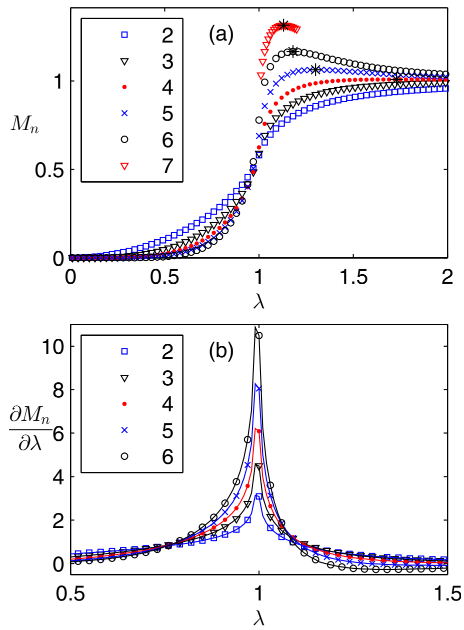

FIG. 2. (Color online) (a) Violation measure of the Mermin inequality for the Ising model ($\gamma = 1$) for $n = 2,\ldots,7$. (b) The derivative of the violation measure of the Mermin inequality for the Ising model ($\gamma = 1$) for $n = 2,\ldots,6$.

of them) should be singular when a phase transition occurs. Thus, it is not a surprising result that $M_n = \mathrm{Tr}(\hat{\rho}_n \hat{M}_n)$ is also singular at the QPT point.

Another signal of the QPT is that M_n shows quite different size effects on the two sides of the critical point. When the size of the subsystem increases, M_n decreases gradually in the region $\lambda < \lambda_c = 1$ and increases steadily for $\lambda > \lambda_c$ [see Fig. 2(a)]. Furthermore, for $\lambda < \lambda_c$, M_n converges very quickly, and the curves for M_5 and M_6 are almost overlapped. For $\lambda > \lambda_c$, however, our results reveal clearly that M_n converges very slowly if, indeed, it can converge. Similar behavior is also observed for $\gamma = 0.6$, as shown in Fig. 3. The results suggest that the ground states on the two sides of $\lambda_c = 1$ are fundamentally different, which can be regarded as a signal of the QPT.

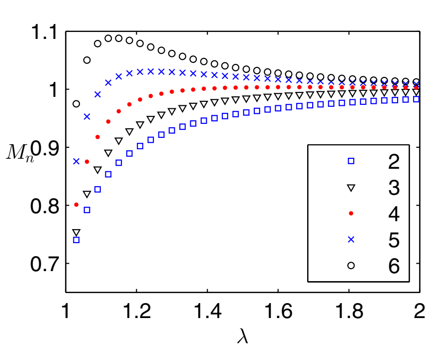

FIG. 3. (Color online) Violation measure of the Mermin inequality as a function of λ of the XY model ($\gamma = 0.6$) for several n.

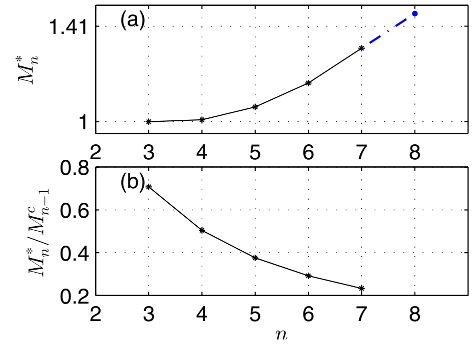

FIG. 4. (Color online) (a) Size dependence of the peak value of M_n of the Ising model ($\gamma = 1$). (b) Size dependence of the genuine n-partite entanglement indicator $\frac{M_n^*}{M_{n-1}^c}$ of the Ising model ($\gamma = 1$). Genuine n-partite entanglement is identified if $\frac{M_n^*}{M_{n-1}^c} > 1$.

C. Multipartite entanglement in the critical region

A direct result of the increase of M_n with n is that, when n is large enough, M_n will present peak points in the vicinity of the critical point. Let's just consider the Ising case as shown in Fig. 2(a). M_2 and M_3 are monotonically increasing functions of λ. For $n = 4,5,6,7$, M_n presents peaks at ($\lambda_4^* = 1.73, M_4^* = 1.008$), ($\lambda_5^* = 1.30, M_5^* = 1.063$), ($\lambda_6^* = 1.18, M_6^* = 1.166$), and ($\lambda_7^* = 1.13, M_7^* = 1.315$), respectively. The peaks are illustrated with asterisks in Fig. 2(a). With the increase of n, the peaks become sharp gradually, and the position of the peaks, i.e., λ_n^*, tends to the critical point $\lambda_c = 1$.

According to the Mermin inequalities (1), (2), and (4), a high value of M_n may result in the violation of these inequalities. Therefore, the peak points of M_n would be valuable in characterizing the multipartite correlation in the system. From Fig. 2(a), one can see that for $n \geqslant 4$ the first-order Mermin inequality $\mathrm{Tr}(\hat{\rho}_n \hat{M}_n) \leqslant 1$ is violated in the vicinity of the peak points. According to the theory in Sec. II, this indicates that at least two-partite entanglement is present in $\hat{\rho}_n$. In fact, the existence of three-partite entanglement can be identified for $n \geqslant 8$. In Fig. 4(a), we display the size dependence of the peak value of M_n, that is, M_n^*. As n increases from 3 to 7, one can see that $\frac{\partial M_n^*}{\partial n}$ increases gradually. It is quite reasonable that $M_8^* > \sqrt{2}$. Therefore, the second-order Mermin inequality $\mathrm{Tr}(\hat{\rho}_n \hat{M}_n) \leqslant \sqrt{2}$ will be violated for $n \geqslant 8$. In other words, at least three-partite entanglement is present for $n \geqslant 8$. Furthermore, since (i) the right-hand side (rhs) of the m-order Mermin inequality [see Eq. (2)] does not depend upon n and (ii) the peak value of left-hand side (lhs) of the inequality, i.e., M_n^*, increases faster and faster as n increases, one can conclude that as long as n is large enough, the arbitrary-order Mermin inequality will be violated. In the framework of m-partite entanglement, multipartite entanglement with an arbitrarily high hierarchy will be observed only if n is large enough.

As we have mentioned, for a large n, the peak of M_n should become sharp and should be located close to the critical point. Thus, high-hierarchy-multipartite entanglement should be present just in the vicinity of the QPT point. In fact, M_n can disclose even more features about the change of the hierarchy of multipartite entanglement in the QPT. When the system moves towards (away from) the critical point, since M_n increases (decreases), the order of the violated inequality will increase (decrease) gradually. In the language of m-partite entanglement, this means that when the system moves towards (away from) the QPT point, the hierarchy of multipartite entanglement in $\hat{\rho}_n$ will increase (reduce).

We have shown that M_n can be used to measure multipartite entanglement. In fact, the size effects in Fig. 2(a) can help us explain the physical meaning of M_n in the context of condensed-matter physics. According to how the correlations decay with distance, a system is usually said to have short-range order (SRO) or long-range order (LRO). If a system is short range correlated, measures of correlations will usually converge fast with the increase of the system size. In Fig. 2(a), the fast convergence of M_n for $\lambda < \lambda_c$ reveals that the correlations in the system are short ranged. On the other hand, LRO is usually detected by the nonconvergence of measures of correlations. For instance, the increase of the structure factor (a well-known tool to study correlations in condensed-matter physics; an example can be found in Ref. [38]) with system size is a widely used signal for LRO. In addition, the nonconvergence of entanglement entropy (a measure of bipartite entanglement) in the QPT is also induced by LRO [7,9,10]. Clearly, the fact that M_n^* increases with n in the vicinity of the critical point is a crucial indicator of the appearance of LRO at the QPT of the XY model. Thus, M_n reveals two significant characteristics of the QPT of the XY model: multipartite correlation and LRO.

D. Multipartite nonlocality in the critical region

In this section, we will analyze the multipartite nonlocality in the XY model with the help of the m-grouping models and the Mermin-Svetlichny inequality (4).

First, we consider the Mermin-Svetlichny inequality where $n - m$ is even. Now the inequality is expressed as $S_n^m = \mathrm{Tr}(\hat{\rho}_n \hat{M}_n) \leqslant 2^{(n-m)/2}$, or, alternatively,

$$M_n \leqslant 2^{(n-m)/2}, \quad \text{for } n - m \text{ even}, \tag{7}$$

which reduces to the Mermin inequality. The Mermin inequality has been extensively studied above; therefore, we are ready to obtain some useful conclusions about the quantum nonlocality. For example, for $n \geqslant 4$, we have already identified the violation of $M_n \leqslant 1 = 2^{0/2}$; thus, the n-order Mermin-Svetlichny inequality will be violated for $n \geqslant 4$. In the grouping-model language, $n - 1$ (or fewer) grouping models are needed to reproduce the nonlocal correlation in $\hat{\rho}_n$ $(n \geqslant 4)$. Furthermore, as suggested by Fig. 2, violation of high-order Mermin inequalities will be observed in the vicinity of λ_c for a large n. Thus, high-hierarchy-multipartite nonlocality will be observed in the vicinity of the critical point.

Second, we consider the Mermin-Svetlichny inequality where $n - m$ is odd, where the inequality is expressed as $S_n^m = \mathrm{Tr}(\hat{\rho}_n \hat{M}_n^+) = M_n^+ \leqslant 2^{(n-m)/2}$. The first nontrivial case is $M_n^+ \leqslant \sqrt{2}$ with $n - m = 1$. A violation of the inequality will indicate that $n - 2$ (or fewer) grouping models are needed to reproduce the nonlocality in the state. In Fig. 5 we have shown M_n^+ for $n = 2, \ldots, 6$ with all $\{\boldsymbol{a}_1, \boldsymbol{a}_1', \ldots\}$ in the x-z plane. One can see that no violation is observed. We have also considered M_n^+ with all $\{\boldsymbol{a}_1, \boldsymbol{a}_1', \ldots\}$ in the x-y plane and y-z plane, and no violation is observed either. In addition, in Fig. 5 only one peak point is observed (in M_6^+); thus, we cannot use the strategy in Fig. 4(a) to make any reliable estimation. This suggests that, to observe the violation of the inequality with an odd $n - m$, a large subsystem is needed.

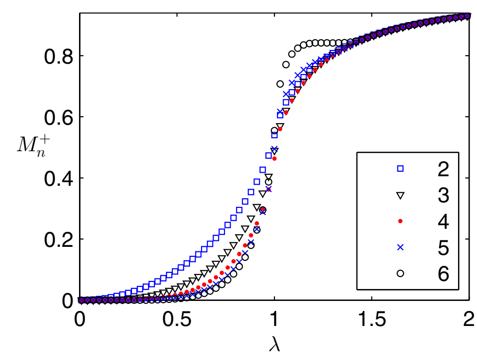

FIG. 5. (Color online) Violation measure of the Mermin-Svetlichny inequality as a function of λ for several n, where $\gamma = 1$ and $n - m$ is odd.

E. Genuine multipartite correlation

Whether or not genuine n-partite correlations would be observed at the QPT point is an interesting topic. First, we consider multipartite entanglement. Let's denote $M_{n-1}^c = 2^{(n-2)/2}$ as the rhs of the $(n-1)$-order Mermin inequality. For some n, if we find $\frac{M_n^*}{M_{n-1}^c} > 1$, the $(n-1)$-order Mermin inequality is violated, and genuine n-partite entanglement is identified. Thus, $\frac{M_n^*}{M_{n-1}^c}$ can be used as an indicator for genuine n-partite entanglement. In Fig. 4(b) we show the size dependence of $\frac{M_n^*}{M_{n-1}^c}$ for $n = 3,4,5,6,7$. One can see that $\frac{M_n^*}{M_{n-1}^c} \leqslant 1$ for all n, and more importantly, $\frac{M_n^*}{M_{n-1}^c}$ decreases gradually. This suggests that genuine n-partite entanglement would not be observed at the QPT point.

Second, we consider genuine multipartite nonlocality. In order to identify genuine n-partite nonlocality, the state $\hat{\rho}_n$ should violate the second-order Mermin-Svetlichny inequality. In the case where n is even, the inequality reduces to $M_n \leqslant 2^{(n-2)/2} = M_{n-1}^c$, or, alternatively, $\frac{M_n}{M_{n-1}^c} \leqslant 1$. As suggested by Fig. 4(b), the violation would never occur. In the case where n is odd, the inequality reduces to $M_n^+ \leqslant 2^{(n-2)/2} = M_{n-1}^c$. As n increases, M_n^+ increases even more slowly than M_n [see Figs. 5 and 2(a)]. Thus, the inequality would not be violated for an odd n either.

These results suggest that genuine n-partite quantum entanglement and nonlocality would not be observed in the XY model by Bell-type experiments [39].

IV. SUMMARY

In this paper, we have studied multipartite quantum correlations in infinite XY chains with an open boundary condition. Specifically, we have used the violation measure M_n

of Bell-type inequalities to evaluate multipartite correlation of an n-spin subsystem located in the middle of the chains.

Some clues for the critical point $\lambda_c = 1$ have been found by analyzing M_n and its derivative $\frac{\partial M_n}{\partial \lambda}$. First, $\frac{\partial M_n}{\partial \lambda}$ is divergent exactly at the critical point for all n. Second, M_n shows quite different size effects on the two sides of the QPT point. Third, as n increases, the position of the peaks, i.e., λ_n^*, approaches the critical point gradually.

The whole interest of this paper is to study how the quantum correlations spread out among the spins when the system undergoes a QPT. It is interesting that M_n can characterize the correlations in the QPT from two different aspects: multipartite correlations in the field of quantum information theory and long-range order in the field of condensed-matter physics. First, we pay attention to the hierarchy of multipartite entanglement and multipartite nonlocality. As long as n is large enough, an arbitrary-order Mermin inequality (and Mermin-Svetlichny inequality) would be violated just at the critical point. Consequently, the n-spin subsystem will show a high hierarchy of multipartite correlation in the vicinity of the QPT point, and the hierarchy of multipartite correlation will reduce gradually when the system moves away from the critical region. We would like to mention that the quantum nonlocality is detected for $n \geqslant 4$ in this paper. It is a meaningful extension of previous studies where quantum nonlocality has not been observed for $n = 2$ in many one-dimensional systems [14–19]. The result shows that in low-dimensional quantum spin models, quantum nonlocality is present naturally in the form of multipartite settings, rather than the bipartite setting. Furthermore, clear evidence shows that genuine n-partite entanglement or genuine n-partite nonlocality cannot be observed in the QPT of the XY model by Bell-type experiments. Moreover, we would like to mention that M_n reveals the long-range correlations in the QPT. With the increase of n, the peak value of M_n does not converge in the vicinity of the critical point, which is a crucial indicator of the appearance of long-range correlations in the QPT.

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[39] Bell inequalities are sufficient but not necessary conditions to witness quantum correlation. Thereby, the XY model may contain other kinds of genuine multipartite correlations which cannot be captured by Bell-type inequalities.