Characterizing entanglement by momentum jump in the frustrated Heisenberg ring at a quantum phase transition

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We study the pairwise concurrences, a measure of entanglement, of the ground states for the frustrated Heisenberg ring to explore the relation between entanglement and quantum phase transition associated with the momentum jump. The ground-state concurrences between any two sites are obtained analytically and numerically. It shows that the summation of all possible pairwise concurrences is an appropriate candidate to depict the phase transition. We also investigate the role that the momentum takes in the jump of concurrence at the critical points. We find that an abrupt momentum change results in the maximal concurrence difference of two degenerate ground states.

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I. INTRODUCTION

A quantum system changes its ground-state properties in a fundamental way when quantum phase transitions (QPTs) occur at absolute zero [1], which are induced by the change of external parameters or coupling constants and are driven by quantum fluctuations. In a finite system the discontinuity of the ground-state energy is often used to characterize the occurrence of QPTs for there is an energy-level crossing at the critical point. We will show, in this paper, that such kind of phase transition is usually accompanied by the change of symmetry characterized by conservative quantities such as the momentum which is the generator of translation. Our investigations will relate to the quantum entanglement measured by the total concurrences [2].

Actually, quantum critical points are governed by a diverging correlation length and there exists a very close relation between quantum correlation and quantum entanglement, which is known as the resource that enables quantum computation and communication. So exploring the role of entanglement in a phase transition has attracted great attention from both the communities of quantum computation and quantum statistics [3–14]. People have connected the theory of critical phenomena with quantum information by exploring the entangling resources of a system close to its quantum critical point. They demonstrate, for a class of magnetic systems or the interacting quantum lattice spin systems at zero temperature, that entanglement shows scaling behavior in the vicinity of the transition point where the level crossing occurs at degenerate ground states [15].

From these studies we observe that the degeneracy of ground states at the critical point may result in the uncertainty of entanglement. This fact means the discontinuity of concurrence in the vicinity of the phase-transition point. Such sudden change of the concurrence as the variation of an external parameter or coupling constant is vividly called the jump of concurrence. However, the ground-state energy-level crossing may not always result in a jump of a certain type of concurrence, such as the next-nearest neighbor (NNN) or other pairwise concurrences. On the other hand, this kind of QPT must be accompanied by a change of a certain conservative quantity, such as the momentum or the macroscopic magnetization. This observation may provide us a different way to find an appropriate definition of concurrence that just characterizes the property of the quantum spin systems at the critical point.

In this paper, we consider a frustrated Heisenberg ring system which contains rich phases in the ground state. To reveal the connection between the concurrence behavior and the symmetries of the separated phases around the critical point, we study the difference between the concurrences of two degenerate ground states at the critical points. We find that there does exist such a discontinuity of a conservative physical quantity momentum (the generator of translation) which results in the maximization of entanglement difference of the two degenerate ground states.

The paper is organized as follows. In Sec. II, the numerical result for the concurrence behavior of a frustrated Heisenberg ring around the critical points is given. It shows that a single type of concurrence is not sufficient to depict a QPT, while the summation of all types of concurrence may be. In Sec. III, the exact results are employed to explain our observation concluded in Sec. II. In Sec. IV, the role that another conservative quantity—momentum—plays in the concurrence jump is studied. The summary and some discussions are given in Sec. V.

II. CONCURRENCE JUMPS IN QPTs

We start from a one-dimensional (1D) frustrated spin-1/2 Heisenberg model with periodic boundary conditions, which belongs to the Majumdar-Ghosh (MG) families of models [16] (see Fig. 1).

The Hamiltonian reads

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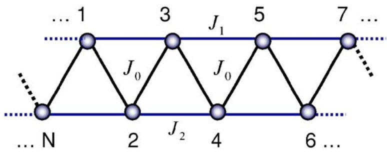

FIG. 1. (Color online) The schematic structure of a frustrated spin-1/2 Heisenberg ring. J_0 denotes the nearest-neighbor coupling constant, while J_1 and J_2 denote the next-nearest-neighbor coupling constants between an even and odd number of sites, respectively. In this paper we are only concerned with the simple case $J_1=J_2=J$.

$$H = J_0\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \tag{1}$$

where N is even denoting the total number of the lattice sites, $\mathbf{S}_i$ is the spin operator at the ith site, and J_0 (J) is the strength of the NN (NNN) exchange interaction. For the periodic boundary conditions, we have $\mathbf{S}_{N+1}=\mathbf{S}_1$. For arbitrary J_0 and J, the ground-state energy of Hamiltonian (1) can be formally written as the function of the parameters J_0 and J,

$$E_g(J_0,J) = J_0h_0 + Jh, \tag{2}$$

in terms of the NN correlation function

$$h_0 = \sum_i \langle g|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|g\rangle \tag{3}$$

and the NNN correlation function

$$h = \sum_i \langle g|\mathbf{S}_i \cdot \mathbf{S}_{i+2}|g\rangle \tag{4}$$

with respect to the ground state $|g\rangle$.

Now we consider the behavior of ground-state energy as the variation of parameters J and J_0. For an infinite system, the energy-level crossing should induce the discontinuity of the derivative of ground-state energy

$$\frac{\partial E_g}{\partial J_0} = \langle g|\frac{\partial H}{\partial J_0}|g\rangle = h_0, \tag{5}$$

which is just the NN correlation function. Since there exists an algebraic relationship between pairwise concurrence and correlation function [17]

$$C_{ij} = \frac{1}{2}\max\{0,|G_{xx}+G_{yy}| - G_{zz} - 1\}, \tag{6}$$

where $G_{\alpha\alpha}=\langle g|\sigma_i^\alpha\sigma_j^\alpha|g\rangle$ ($\alpha=x,y,z$) are correlation functions, then according to Eq. (5) the energy-level crossing will lead to the discontinuity of the NN concurrence. On the other hand, one can also establish a similar relation between NNN correlation function h and the discontinuity of $\partial E_g/\partial J$,

$$\frac{\partial E_g}{\partial J} = \langle g|\frac{\partial H}{\partial J}|g\rangle = h. \tag{7}$$

Notice that, for nonzero J_0, if the correlation h has a jump due to the discontinuity of $\partial E_g/\partial J$, the other correlation function h_0 must experience a jump at the same point $J=J_c$. Actually, at the energy-level crossing point the ground states are degenerates, i.e.,

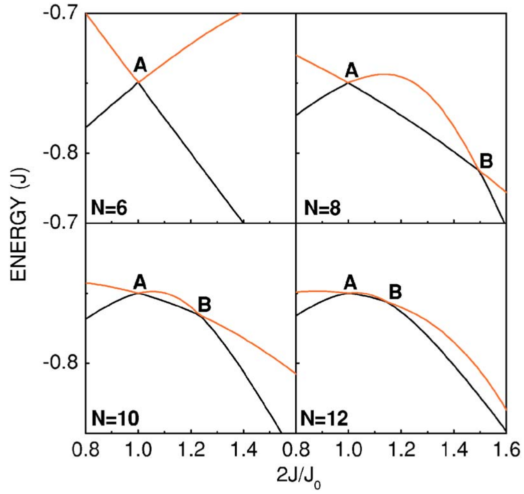

FIG. 2. (Color online) The ground and first excited eigenenergies for the systems of the size $N=6$, 8, 10, and 12. A and B denote the energy-level crossing points where the quantum phase transitions occur. The critical point A is always at $J=J_c=J_0/2$, while the position of point B depends on the size of the system.

$$J_0h_0 + Jh = J_0h_0' + Jh', \tag{8}$$

where

$$h_0' = \sum_i \langle g'|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|g'\rangle,$$

$$h' = \sum_i \langle g'|\mathbf{S}_i \cdot \mathbf{S}_{i+2}|g'\rangle \tag{9}$$

are the corresponding correlations with respect to another ground state $|g'\rangle$. No doubt, both the NN and NNN correlation functions must be discontinuous or have jumps at critical point $J=J_c$. But the jump of one type of correlation may not necessarily induce the jump of its corresponding concurrence. A natural question is, which type of concurrence, NN or NNN, plays a major role in depicting the QPTs at the critical points? To answer this question, we investigate the frustrated spin-1/2 Heisenberg ring numerically and analytically. In Fig. 2, the eigenenergies of the ground and first excited state are plotted for the systems with size $N=6$, 8, 10, and 12. A and B denote the two energy-level crossing points.

The reduced density matrix for two spins located at sites i and j [18] has the form

$$\rho_{ij} = \begin{pmatrix} v_{ij} & 0 & 0 & 0 \\ 0 & w_{ij} & z_{ij} & 0 \\ 0 & z_{ij} & w_{ij} & 0 \\ 0 & 0 & 0 & v_{ij} \end{pmatrix} \tag{10}$$

with respect to the standard basis vectors $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$. Correspondingly the concurrence can be calculated by

TABLE I. The jumps of the pairwise concurrences $C^{[\alpha]}$ and total concurrence C_T at the critical point B for the $N=8$, 10, and 12 systems. It implies that not all types of concurrence are appropriate to depict the QPTs, while the total concurrence is an appropriate one.

N	8	10	12
$\alpha=1$	0.7660	1.2755	0.6228
$\alpha=2$	1.8228	0	0
$\alpha>2$	0	0	0
Total	1.0568	1.2755	0.6288

$$C_{ij}=\max\{0,2(|z_{ij}|-v_{ij})\}.$$

Furthermore, for the ground state with vanishing total spin, it can be connected to the isotropic correlation function $\langle\sigma_i\cdot\sigma_j\rangle$ by [17]

$$C_{ij}=\frac{1}{2}\max\{0,-\langle\sigma_i\cdot\sigma_j\rangle-1\}. \tag{11}$$

Analytical and numerical results show that the ground states of the Hamiltonian (1) for the sizes we concern have spin zero. Then the concurrences can be obtained directly from the corresponding correlation functions. Now we define the α type concurrence

$$C^{[\alpha]}=\sum_i^{N-1}C_{i,i+\alpha}, \tag{12}$$

where $\alpha=1,2,\ldots,N/2$, and the total concurrence as the summation of all types of concurrences, i.e.,

$$C_T=\sum_\alpha^{N/2}C^{[\alpha]}. \tag{13}$$

It is obvious that C_T shares the same property as the average concurrence [19]. We also define the concurrence jump as $\Delta^{[\alpha]}=|C_L^{[\alpha]}-C_R^{[\alpha]}|$ ($\Delta_T=|C_{TL}-C_{TR}|$) denoting the α (total) type concurrence difference between the two ground states at the left (L: $J=J_c-0^+$) and right (R: $J=J_c+0^+$) side of the critical points.

The conjectures of the relationship between entanglement and QPTs in Refs. [1,14] tell us that the concurrence, a measure of entanglement, should be changed largely at the critical points. So we calculate concurrence at point B, for $N=8$, 10, and 12 systems numerically. The corresponding concurrence jumps $\Delta^{[\alpha]}$ and Δ_T are listed in Table I.

The big concurrence jumps $\Delta^{[1]}$ for $N=8$, 10, 12 and $\Delta^{[2]}$ for $N=8$ match the energy-level crossing in Fig. 2, while the rest concurrences show no special behavior at point B. It indicates that, at the critical point, not all types of concurrence change largely. It shows that different types of concurrences show different behaviors around the critical points. It seems that there exists no single preferable type of concurrence in characterizing the QPTs. A natural way to treat this problem is to use the summation of all types of concurrence. In the following section, we will investigate the critical behavior at point A . The results further demonstrate that the total concurrence C_T seems to be a good candidate to depict the QPTs.

III. MOMENTUM JUMP IN QPTS CHARACTERIZED BY ENTANGLEMENT

According to quantum mechanics, we can always find out a conservative quantity to distinguish the two degenerate ground states at the energy-level crossing point. In this section we study the critical behaviors at the energy-level crossing points A and B (Fig. 2). We will show that these critical points are just between the phases with momenta 0 and π.

In the case $J=J_0/2$, the exact ground states of the N site system can be explicitly expressed as

$$|\phi_1\rangle=[12][34]\cdots[N-1\ N] \tag{14}$$

or

$$|\phi_2\rangle=[23][45]\cdots[N1] \tag{15}$$

which are the direct products of the resonant valence bond (RVB) states $[ij]=(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2}$ of two spins located at the lattice sites i and j [20]. Obversely, $|\phi_1\rangle$ and $|\phi_2\rangle$ are not orthogonal except in the case of thermodynamical limit, but their combinations $|\phi_1\rangle-|\phi_2\rangle$ and $|\phi_1\rangle+|\phi_2\rangle$ are two orthogonal degenerate ground states.

Because the Hamiltonian is invariant under the translational transformation T, where $T|\uparrow\rangle_i=|\uparrow\rangle_{i+1}$, the common eigenstates $|\psi\rangle=|\psi(\mathbf{S}_1,\mathbf{S}_2,\ldots,\mathbf{S}_N)\rangle$ of H and T have momentum

$$k=\frac{2\pi n}{N}\equiv na,\quad n=1,2,\ldots,N$$

which satisfies $T|\psi\rangle=\exp(ina)|\psi\rangle$. Actually as mentioned above, at point $J=J_0/2$, one can construct the two degenerate ground states as

$$|\psi_1\rangle=\frac{1}{\sqrt{\Omega_1}}[|\phi_1\rangle-|\phi_2\rangle],$$

$$|\psi_2\rangle=\frac{1}{\sqrt{\Omega_2}}[|\phi_1\rangle+|\phi_2\rangle], \tag{16}$$

with momentum $k=0$ and π, respectively. Here

$$\Omega_1=\langle\phi_1|\phi_1\rangle+\langle\phi_2|\phi_2\rangle-2\,\mathrm{Re}(\langle\phi_1|\phi_2\rangle),$$

$$\Omega_2=\langle\phi_1|\phi_1\rangle+\langle\phi_2|\phi_2\rangle+2\,\mathrm{Re}(\langle\phi_1|\phi_2\rangle)$$

are the normalization factors.

We take a system of small size as an analytical illustration for the momentum jump in QPT. For the system of $N=6$, the ground states of the Hamiltonian can be obtained exactly in the whole range of J as

$$|\psi_g\rangle=\begin{cases}|\psi_1\rangle & (J\geqslant J_0/2)\\ (|\psi_2\rangle+\eta|\psi_e\rangle)/\sqrt{\Omega_3} & (J\leqslant J_0/2)\end{cases} \tag{17}$$

corresponding to the eigenvalues

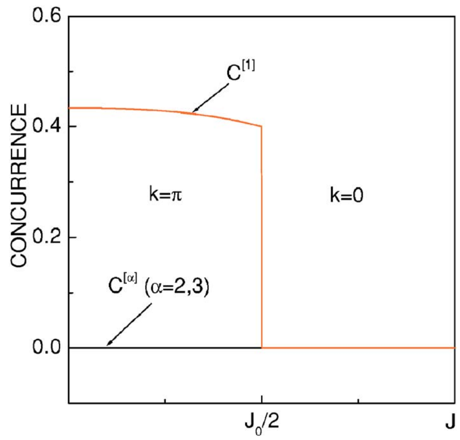

FIG. 3. (Color online) Various types of concurrence as the function of J for $N=6$. The momenta of the ground state for $J<J_0/2$ and $J>J_0/2$ are π and 0 respectively. It shows that only the NN type of concurrence possesses a jump around the critical point $J=J_0/2$.

$$E_1 = -3(J_0+J)/2,$$

$$E_2 = (\eta - 5/2)J_0 + (1/2 - \eta)J, \tag{18}$$

respectively. Here

$$\Omega_3 = 8\eta^2 - 8\eta + 20,$$

$$\eta = \frac{J - 3J_0 + \sqrt{9J^2 - 18JJ_0 + 13J_0^2}}{2(J-J_0)}, \tag{19}$$

and

$$|\psi_e\rangle = \frac{1}{2\sqrt{2}}[(1 - T + T^2 - T^3 + T^4 - T^5)|\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle - (1-T)|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle], \tag{20}$$

is the excited state of the Hamiltonian (1) for $J=J_0$ with eigenenergy 0 and momentum π. It is easy to find that there is only one critical point at which the energy-level crossing occurs. But for $N>6$, there is one more energy-level crossing point at $J>J_0/2$ as illustrated in Fig. 2.

Based on the exact results, the two spin concurrences are obtained as

$$C^{[1]} = \begin{cases} -4(\eta^2 + 2\eta - 2)/\Omega_3 & (J < J_0/2) \\ 0 & (J > J_0/2) \end{cases} \tag{21}$$

and

$$C^{[\alpha]} = \begin{cases} 0 & (J < J_0/2) \\ 0 & (J > J_0/2) \end{cases} \qquad (\alpha = 2,3), \tag{22}$$

which are plotted in Fig. 3.

It shows that the NN concurrence $C^{[1]}$ has a jump at the critical point A, while other types of concurrences $C^{[\alpha]}$ ($\alpha>1$) do not have any special behavior. Obviously C_T also has a jump at the critical point, which is in agreement with the observation presented in Sec. II. In the following section, we will investigate the relations between various types of concurrence jumps and a conservative quantity, momentum, which has a jump for the QPTs.

IV. CONCURRENCE JUMP IN ASSOCIATION WITH MOMENTUM JUMP IN QPT

From the above analysis, we know that the jumps of concurrences $C^{[\alpha]}$ at the critical points may be induced by the energy-level crossing or the discontinuity of the ground-state energy as a function of the coupling constants. On the other hand, at the energy-level crossing point, the ground states are degenerate. Thus an arbitrary linear combination of two degenerate ground states is also the ground state. If a certain type of concurrence has a jump at the critical point, the corresponding concurrence of the combined ground state should be uncertain. Meanwhile the difference of the concurrences between the two orthogonal combined ground states should also depend on the way of the combination. On the other hand, as the energy-level crossing there must exist a conservative quantity which also experiences a jump. Then the phase separation can be also well described in association with the jump of such a quantity. In this paper, this conservative quantity is *momentum* which is the generator of translation. In general, one may say that the discontinuity of $\partial E_g/\partial J$ leads to the jump of concurrence at the critical points, but on the other hand, one can also say that it is the discontinuity of *momentum* of the ground state that leads to the jump of concurrence at the critical point.

In order to investigate the role that the momentum plays on the change of various types of concurrence $C^{[\alpha]}$, we reconstruct two degenerate ground states at the critical point A as

$$|\Psi_1\rangle = \cos\frac{\theta}{2}|\psi_1\rangle + e^{i\phi}\sin\frac{\theta}{2}|\psi_2\rangle,$$

$$|\Psi_2\rangle = e^{-i\phi}\sin\frac{\theta}{2}|\psi_1\rangle - \cos\frac{\theta}{2}|\psi_2\rangle, \tag{23}$$

where $\theta\in[0,\pi]$ and $\phi\in[0,2\pi]$. For N-site systems ($N\geqslant 6$), the pairwise concurrences of type α (total concurrence) of the two degenerate ground states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are denoted as $C_1^{[\alpha]}$ and $C_2^{[\alpha]}$ (C_{T1} and C_{T2}), respectively. A straightforward calculation shows that $C_1^{[\alpha]}=C_2^{[\alpha]}=0$ for $\alpha>1$, while $C_1^{[1]}$ and $C_2^{[1]}$ are nonzero and depend on the parameters θ and ϕ. Obviously, states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are no more the eigenstates of momentum in the general case.

What we concern is the role the momentum plays on the jump of the concurrence. For $N>6$ the difference between $C_1^{[1]}$ and $C_2^{[1]}$ is

$$|C_1^{[1]} - C_2^{[1]}| = |\varepsilon_{11} + \varepsilon_{12} - \varepsilon_{21} - \varepsilon_{22}|, \tag{24}$$

where

$$\varepsilon_{ij} = \frac{1}{4}H(3G_{ij}-1)(3Q_{ij}-1), \tag{25}$$

$$Q_{ij} = 1 - 2\chi_N^2 + (-)^i \xi_N \chi_N^2 \cos\theta + (-)^{i+j}\chi_N \cos\phi \sin\theta, \tag{26}$$

$$\chi_N \equiv [4-\xi_N^2]^{-1/2}, \quad \xi_N \equiv \left(\frac{1}{2}\right)^{N/2-2} \tag{27}$$

and

$$H(x) = \begin{cases} 1 & (x>0) \\ 0 & (x<0) \end{cases} \tag{28}$$

is the Heaviside step function. In the following, we will show that this difference reaches maxima at $\theta=0,\pi$ for any $\phi \in [0,2\pi]$.

Notice that $3Q_{ij}-1 \geqslant 0$ always holds when $\phi=\pi/2$, $3\pi/2$. Then Eq. (24) can be rewritten as

$$|C_1^{[1]} - C_2^{[1]}| = 3|\xi_N \chi_N^2 \cos\theta|. \tag{29}$$

It is a monotonic function, which reaches its maxima at $\theta=0,\pi$.

Now we prove that for any θ, the inequality

$$|C_1^{[1]} - C_2^{[1]}| \leqslant 3|\xi_N \chi_N^2 \cos\theta| \tag{30}$$

holds in all the range of ϕ. It is convenient to consider the problem in the range $\theta,\phi \in [0,\pi/2]$ without loss of generality. Since the functions $\sin\theta$, $\cos\theta$, and $\cos\phi$ are positive in this range, we can prove the above conclusion in the following three cases.

Case 1:

$$3Q_{12}-1 = A - 3\chi_N \cos\phi \sin\theta > 0,$$

$$3Q_{21}-1 = B - 3\chi_N \cos\phi \sin\theta > 0; \tag{31}$$

case 2:

$$3Q_{12}-1 = A - 3\chi_N \cos\phi \sin\theta < 0,$$

$$3Q_{21}-1 = B - 3\chi_N \cos\phi \sin\theta > 0; \tag{32}$$

case 3:

$$3Q_{12}-1 = A - 3\chi_N \cos\phi \sin\theta < 0,$$

$$3Q_{21}-1 = B - 3\chi_N \cos\phi \sin\theta < 0, \tag{33}$$

where we have defined

$$A = 2 - 6\chi_N^2 - 3\xi_N\chi_N^2 \cos\theta > 0,$$

$$B = 2 - 6\chi_N^2 + 3\xi_N\chi_N^2 \cos\theta > 0,$$

$$B \geqslant A. \tag{34}$$

For all the above three cases we have

$$3Q_{11}-1 = A + 3\chi_N \cos\phi \sin\theta > 0,$$

$$3Q_{22}-1 = B + 3\chi_N \cos\phi \sin\theta > 0. \tag{35}$$

Actually, in case 1, we have

$$|C_1^{[1]} - C_2^{[1]}| = 3|\xi_N \chi_N^2 \cos\theta|.$$

In case 2, from Eq. (32) we have

$$|D| < |-4\xi_N\chi_N^2 \cos\theta|, \tag{36}$$

where

$$D = -\frac{2}{3} - 3\xi_N\chi_N^2 \cos\theta + \chi_N \cos\phi \sin\theta + 2\chi_N^2. \tag{37}$$

Then the concurrence difference is

$$|C_1^{[1]} - C_2^{[1]}| = |\varepsilon_{11} - \varepsilon_{21} - \varepsilon_{22}| = \frac{3}{4}|D| < 3|\xi_N\chi_N^2 \cos\theta|. \tag{38}$$

Similarly, for case 3, we have

$$|C_1^{[1]} - C_2^{[1]}| = \frac{3}{2}|\xi_N\chi_N^2 \cos\theta| < 3|\xi_N\chi_N^2 \cos\theta|. \tag{39}$$

For the cases that θ and ϕ are taken in the rest ranges, a similar proof as presented in Eqs. (31)–(39) can get the same conclusion. So from Eqs. (29) and (30) we conclude that the concurrence difference between $C_1^{[1]}$ and $C_2^{[1]}$ reaches the maxima when $\theta=0,\pi$ for any ϕ.

In fact, for the cases $N \geqslant 8$ within the special domain of $\theta \sim 0,\pi$ and any ϕ, it always holds that $3Q_{ij}-1>0$. Hence we have

$$|C_1^{[1]} - C_2^{[1]}| = \begin{cases} 3\xi_N\chi_N^2(1-\theta^2) & (\theta \sim 0) \\ 3\xi_N\chi_N^2[1-(\pi-\theta)^2] & (\theta \sim \pi) \end{cases} \tag{40}$$

which reaches its maxima $3\xi_N\chi_N^2$ at $\theta=0,\pi$. Here the two combined states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are just the eigenstates of momentum, i.e., the ground states at $J=J_c \pm 0^+$.

As illustration, in Fig. 4 the concurrence differences, $|C_1^{[\alpha]} - C_2^{[\alpha]}|$ as the functions of the parameters θ and ϕ are plotted for $N=6$, 8, 12, and 16 systems.

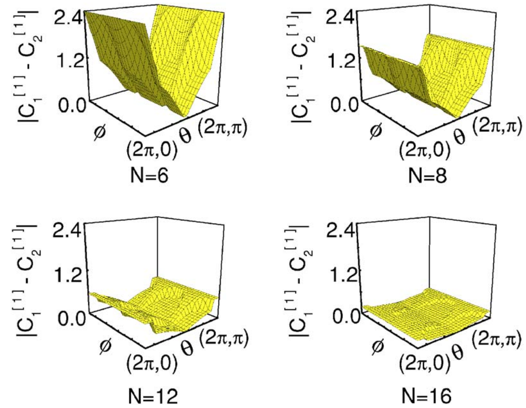

FIG. 4. (Color online) The NN concurrence difference of the two reconstructed degenerate ground states for $N=6$, 8, 12, and 16. Since all the rest types of concurrences are 0, the behavior of $|C_1^{[1]} - C_2^{[1]}|$ and $|C_{T1} - C_{T2}|$ are the same. It shows that the total concurrence difference reaches the maxima when $\theta=0$ or π for all ϕ and N, but the maxima decay exponentially with the size N of the system.

It shows that there always exists a maximal concurrence difference, or a maximal concurrence jump, at the points where the two degenerate ground states are the eigenstates of momentum with $k=0,\pi$. Furthermore, in the thermodynamic limit, we have $\lim_{N\to\infty}\xi_N=0$ and $\lim_{N\to\infty}\chi_N=1/2$, and then the maxima decays to zero exponentially. The results indi-

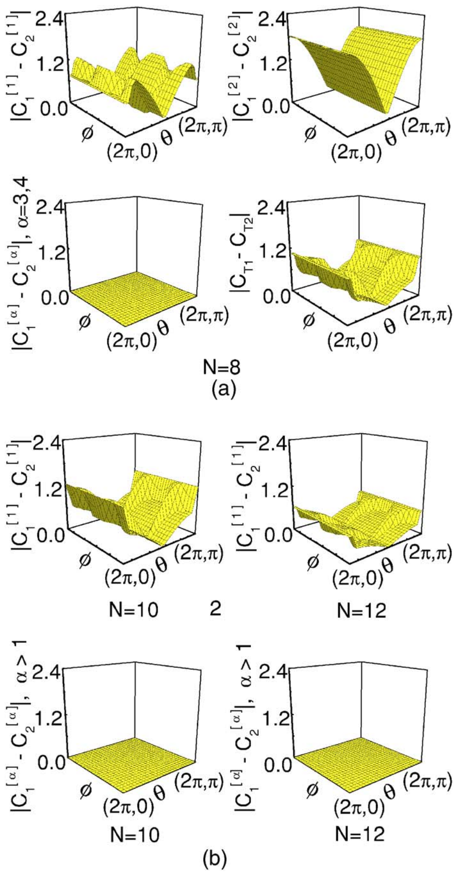

FIG. 5. (Color online) All types of concurrence differences of the degenerate ground states for $N=8$ (a) and 10, 12 (b). Notice that the anomalous behavior in the $N=8$ case shows that only the total concurrence difference reaches the maxima when $\theta=0$ or π for all ϕ and N.

cate that the change of the momentum induces the maximal jump of $|C^{[1]}|$ or $|C_T|$ at point A. So far, we cannot say which type of concurrence is preferable to characterize the QPT; from the following arguments, we will see that an anomalous result for point B will give a final selection.

Now we turn to consider the situation at the critical point B. In this case, the differences of concurrence $|C_1^{[\alpha]}-C_2^{[\alpha]}|$ and $|C_{T1}-C_{T2}|$ cannot be obtained analytically. The numerical method is employed to calculate the differences of various types of concurrences. All types of concurrence difference as the functions of the parameters θ and ϕ are plotted in Fig. 5.

In Fig. 5(a), it shows that the pairwise concurrences of NN and NNN for $N=8$ have jumps, while the rest have no jumps. This result is different from that for the A point, in which case there is no jump for NNN concurrence. Another interesting result is that the difference $|C_1^{[1]}-C_2^{[1]}|$ does not reach the maxima when the corresponding two degenerate states are the eigenstates of momentum. This anomalous phenomenon indicates that the NN concurrence seems not to be sufficient to characterize the QPT. However, Fig. 5(a) also shows that the difference $|C_{T1}-C_{T2}|$ still obeys the same rule we obtained at point A. In Fig. 5(b) the corresponding results for $N=10$ and 12 are plotted, which are similar to that of point A. Thus all the results imply that the difference of total concurrence reaches the maxima when two degenerate states are the eigenstates of momentum. In other words, it is the change of momentum that induces the jump of total concurrence. Based on all the results, we conclude that the total concurrence is a good candidate to characterize the quantum critical behavior for the frustrated spin-ring systems concerned.

V. DISCUSSION

Summing up, in this paper we have shown how to establish the connection between the concurrence jump and the change of ground-state momentum at the QPT critical point. All types of pairwise concurrence are investigated analytically and numerically. The results for both critical points A and B indicate that the difference of total concurrence reaches the maxima when the two degenerate ground states are just the eigenstates of momentum. It also reveals another interesting relation between the correlation function and the concurrence. As mentioned in Sec. II, the NN and NNN correlation function must have a jump at the energy-level crossing points, while the NN and NNN concurrences may not. But when the total concurrence is considered, it must have a jump at the critical points. However, the total correlation function $\Sigma_{ij}\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle_g=1/2\langle(\mathbf{S}^2-\Sigma_i\mathbf{S}_i^2)\rangle_g$ (where $\mathbf{S}=\Sigma_i\mathbf{S}_i$ is the total spin) has no jump at the critical points since the spins of the ground states are zero.

Concerning the model for the case $J_1\neq J_2$ as illustrated in Fig. 1, a straightforward calculation shows that the states $|\psi_1\rangle$ and $|\psi_2\rangle$ defined in Eq. (16) are still the degenerate ground states of the Hamiltonian if $J_1+J_2=J_0$. This means that $J_1+J_2=J_0$ is the boundary of different quantum phases in the J_1-J_2 plane. Starting from this observation we can extend our study to the more general case of $J_1\neq J_2$ to verify the conclusion obtained in this paper. It will appear in a successive paper.

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