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# Reduced fidelity and quantum phase transitions in spin-1/2 frustrated Heisenberg chains

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## Abstract

We use reduced fidelity to characterize quantum phase transitions in the one-dimensional spin-1/2 antiferromagnetic Heisenberg chain with frustration. For the ground state and the low-lying excited states, explicit results of the reduced fidelities between the nearest-neighbor and next-nearest-neighbor spins are given in both the even-size and odd-size cases. We find the reduced fidelity is an effective tool in detecting the quantum phase transitions associated with level crossings for the finite-size systems. Interestingly, the reduced fidelity between next-nearest-neighbor spins is evidently more sensitive at the quantum phase transition points than the nearest-neighbor case. Moreover, the reduced fidelity of the low-lying excited states is a good indicator both for the first-order and infinite-order quantum phase transitions of the system.

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## 1. Introduction

Fidelity, which describes the overlap between two states, has been recently introduced from the quantum-information theory to characterize quantum phase transitions (QPTs) [1]. Since QPTs are induced by the changes of external parameters at zero temperature, the ground-state (GS) fidelity [2–5], i.e., the overlap of GS corresponding to slightly different external parameters, becomes a successful tool in measuring QPTs. This has been proved in XY spin chains and Dicke model [3], XXZ chain [6], Hubbard model [7, 8], frustrated Heisenberg chain [9], the heteronuclear molecular Bose–Einstein-condensate model [10], Kitaev honeycomb model [11], extended Harper model [12] and matrix product states [13]. The main advantage of fidelity as an indicator of QPTs is that it is a purely Hilbert-space geometrical quantity and does not need *a priori* knowledge of the order parameter, which is a traditional notation of QPTs and generally not easy to be found for a given system. However, all the above works are concentrated on the fidelity of the global system, while the subsystems are indeed

of more practical use in experiments. Therefore, reduced fidelity (RF) (or named partial fidelity) is naturally introduced to describe the overlap of the GS for the subsystem under a global changed parameter, and has been proved to be as effective as the fidelity of global systems, like the XY model [14, 15], BCS superconductor [16], Lipkin–Meshkov–Glick model [17, 18], dimerized Heisenberg chain [19] and bilinear–biquadratic model [20]. In addition, there is another important quantum-information concept, entanglement, which is studied extensively in previous works [21–24], and is shown to be effective in detecting QPTs. However, we emphasize that, the reduced fidelity, which describes the overlap between states, is more direct in physical motivation and implication.

In our previous work [19], we have investigated the RF for the antiferromagnetic Heisenberg chain with dimerization, i.e., inhomogeneous nearest-neighbor (NN) spin coupling. We find that the RF between NN couplings is an effective indicator for the second-order QPT of the system. On the other hand, the Heisenberg chain with frustration, i.e., next-nearest-neighbor (NNN) spin coupling, is another interesting quantum many-body system for the existence of competition between NN and NNN couplings. It well describes the material structure in some quasi-one-dimensional (quasi-1D) compounds, such as  $\text{CuGeO}_3$  [25, 26] and  $\text{NaV}_2\text{O}_5$  [27]. Therefore, it is an intriguing issue to investigate the RF for the QPTs of such a system [28–32]. There are two important QPTs in this model, a first-order QPT and an infinite-order QPT. The first-order QPT point is easily manifested by the quantum-information concepts like GS entanglement [28–30] and operator fidelity susceptibility [31], while the infinite-order QPT is more convenient to be determined by the information of the low-lying excited states (ESs) like the first ES fidelity [32]. The explanations will be given in section 2.1. It is noted that most of the above works are focused on the systems with even size, since in these cases the results always converge fast to the QPT points. Furthermore, for the odd-size systems, the GSs are generally degenerate and the energy structure of ESs becomes rather complex. As yet, there are very few works [31] concerning about the QPTs in the odd-size systems.

In this work, we will use the RF to study QPTs of the 1D spin-1/2 antiferromagnetic Heisenberg chain with frustration. It is interesting to find that the RF between NNN spins is evidently more sensitive at the QPT points than that between NN spins, and the RF for the low-lying ES is also an effective indicator of QPTs of this system both for even- and odd-size cases.

This paper is organized as follows. In section 2, we introduce the model, derive a general expression of RF, and discuss the energy spectra of the system. In section 3, the QPTs of the system is studied analytically and numerically. Finally, a summary is presented in section 4.

## 2. Reduced fidelity and energy spectra

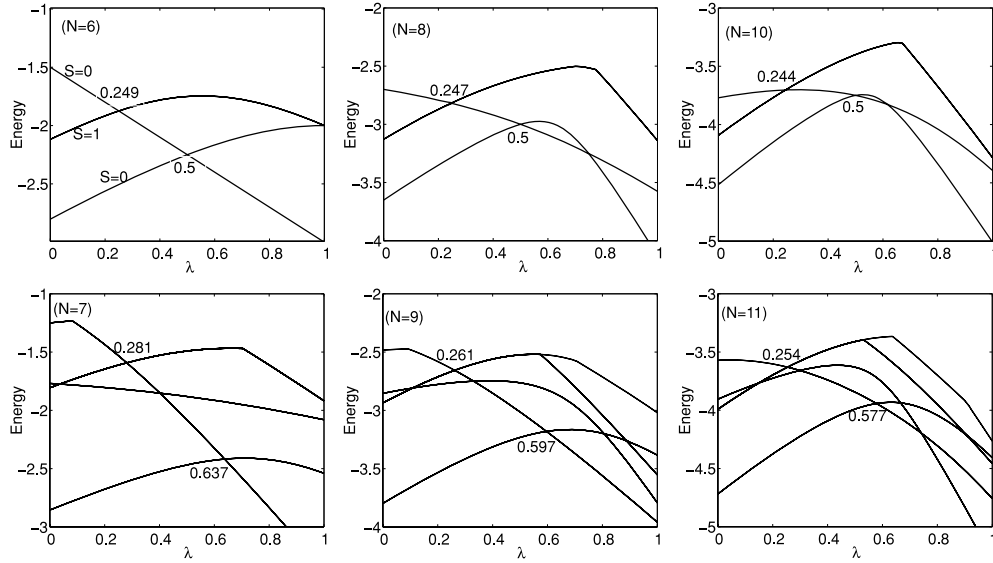
### 2.1. Model

The Hamiltonian for the antiferromagnetic Heisenberg chain with frustration reads [33]

$$H = \sum_{i=1}^N (\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \lambda \mathbf{S}_i \cdot \mathbf{S}_{i+2}), \quad (1)$$

where  $\mathbf{S}_i$  denotes the  $i$ th spin-1/2 operator,  $\lambda > 0$  is the ratio between NNN and NN couplings. The periodic boundary condition  $\mathbf{S}_1 = \mathbf{S}_{N+1}$  is assumed.

It is known that there are two important QPT points of this system, i.e.,  $\lambda_{1c} = 0.5$  and  $\lambda_{2c} \simeq 0.241$ .



**Figure 1.** Low-lying energy spectra for  $N = 6, 8, 10$  and  $N = 7, 9, 11$  of the frustrated Heisenberg chain in the antiferromagnetic case.

(i) At  $\lambda_{1c} = 0.5$ , the system reduces to an exactly solvable model, i.e., Majumdar–Ghosh model [34, 35]. Its GS is of spin zero, but degenerate, which is a uniformly weighted superposition of two NN valence bound states (for even and infinite  $N$  cases)

$$\begin{aligned}
 |\varphi_R\rangle &= [1, 2][3, 4] \cdots [N - 1, N], \\
 |\varphi_L\rangle &= [N, 1][2, 3] \cdots [N - 2, N - 1],
 \end{aligned}
 \tag{2}$$

where  $[i, j] = (|0_i\rangle|1_j\rangle - |1_i\rangle|0_j\rangle)/\sqrt{2}$ . The corresponding GS energy per spin is  $-3/4$ . This point is just the GS energy-level crossing induced by the translation symmetry breaking [36]. Thus it is a first-order QPT point. Using the quantum-information concepts, it is able to be detected by GS concurrence [28, 29], entanglement entropy [30] and operator fidelity susceptibility [31], etc.

(ii) At  $\lambda_{2c} \simeq 0.241$ , the system undergoes a Berezinskii–Kosterlitz–Thouless (BKT) type QPT from spin fluid to dimerized phase [37–39]. This phase transition is driven by the competition between the NN and NNN interactions. When  $\lambda < \lambda_{2c}$ , the NNN interaction does not change the character of the simple antiferromagnetic case  $\lambda = 0$ , whose GS is described as spin fluid massless spinon excitations. When  $\lambda > \lambda_{2c}$ , the frustration term is relevant and the GS flows to the strong-coupling dimerized phase. Furthermore, it is found that  $\lambda_{2c}$  is accurately the degenerate point of the first-excited singlet and triplet states for even-size and infinite-size cases [40–43]. As shown in figure 1, the gap between the GS and the low-lying ESs scales as the system size as  $1/N$ . For  $\lambda < \lambda_{2c}$ , the energy of the singlet state (with total spin  $S = 0$ ) is higher than the triplet state ( $S = 1$ ). For  $\lambda > \lambda_{2c}$ , the singlet state becomes degenerate with the GS as  $N \rightarrow \infty$ , and an energy gap between the triplet state and the two GSs is formed accompanied by the stabilization of a dimerized phase. Therefore, many works were done based on this fact and proved it as a reliable method to obtain  $\lambda_{2c}$  [32, 44]. For example, [32] has proposed the fidelity of the first ES to be an indicator of this  $\lambda_{2c}$ . There are also studies [45] showing that when the GS is known to be nondegenerate, the QPTs are

actually caused by the reconstructions of ESs of the Hamiltonian. In this work, we will use the RF of the lowing-lying ESs to detect this point.

## 2.2. Reduced fidelity

The GS fidelity is defined as [2–5]

$$F = |\langle \Psi(\lambda) | \Psi(\lambda + \delta) \rangle|, \quad (3)$$

where  $|\Psi(\lambda)\rangle$  represents the global GS of the system, and  $\delta$  is a small change of the system parameter  $\lambda$ . Here, the GS is a pure state. However, for a subsystem, it becomes a mixed one, since some of the degrees of freedom of the system is traced out. In this case, it is convenient to use the definition of mixed-state fidelity [47, 48]

$$F = \text{tr} \sqrt{\rho(\lambda)^{1/2} \rho(\lambda + \delta) \rho(\lambda)^{1/2}}, \quad (4)$$

with  $\rho(\lambda)$  the reduced density matrix of the GS. The definitions of (3) and (4) are also applicable to ESs.

It is noted that the Hamiltonian (1) has the SU(2) symmetry, i.e.,  $[H, S_\alpha] = 0$  with  $S$  the total spin and  $\alpha = x, y, z$ . This guarantees the reduced density matrix between two arbitrary spins  $i$  and  $j$  has the form [46]

$$\rho_{ij} = \text{diag}(\varrho_1, \varrho_2), \quad (5)$$

with

$$\varrho_1 = \begin{pmatrix} u^+ & 0 \\ 0 & u^+ \end{pmatrix}, \quad \varrho_2 = \begin{pmatrix} u^- & w \\ w & u^- \end{pmatrix}, \quad (6)$$

in the basis  $\{|00\rangle, |11\rangle, |01\rangle, |10\rangle\}$ , where  $\sigma_z|0\rangle = -|0\rangle$  and  $\sigma_z|1\rangle = |1\rangle$ . The matrix elements are given by

$$u^\pm = \frac{1}{4}(1 \pm c_{ij}), \quad w = \frac{1}{2}c_{ij}, \quad (7)$$

with  $c_{ij} = \langle \sigma_{iz} \sigma_{jz} \rangle = \text{tr}(\rho_{ij} \sigma_{iz} \sigma_{jz})$ . This means that the reduced density matrix  $\rho_{ij}$  is only related to the spin correlator  $c_{ij}$ . In addition, there is an exchange invariance in the Hamiltonian, which leads to the facts that, any two terms of the form  $c_{i,i+1}$  equal to each other, so are the terms  $c_{i,i+2}$ . Thus, in this paper, we only consider the reduced density matrices with the NN and NNN couplings, i.e.,  $\rho_{12}$  and  $\rho_{13}$ .

It is noted that both  $\varrho_1$  and  $\varrho_2$  in equation (6) are Hermitian, and can be rewritten in terms of Pauli operators as  $\varrho_1 = u^+ I$ ,  $\varrho_2 = u^- I + w \sigma_x$ , where  $I$  denotes a  $2 \times 2$  identity matrix. Subsequently, it is found that  $\varrho_i \equiv \varrho_i(\lambda)$  ( $i = 1, 2$ ) commutes with  $\tilde{\varrho}_i \equiv \varrho_i(\lambda + \delta)$  with  $\delta$  a small change of the system parameter  $\lambda$ , i.e.,  $[\varrho_i, \tilde{\varrho}_i] = 0$ . Thus they can be diagonalized simultaneously. With the definition in equation (4), we get [19, 20]

$$F_{\varrho_i} = \text{tr} \sqrt{\varrho_i^{1/2} \tilde{\varrho}_i \varrho_i^{1/2}} = \text{tr} \sqrt{\varrho_i \tilde{\varrho}_i} = \sum_j \sqrt{\lambda_j \tilde{\lambda}_j}, \quad (8)$$

where  $\lambda_j$ s and  $\tilde{\lambda}_j$ s are the eigenvalues of  $\varrho_i$  and  $\tilde{\varrho}_i$ , respectively. This result indicates that if  $\varrho_i$  commutes with  $\tilde{\varrho}_i$ , then  $F_{\varrho_i}$  is only determined by the eigenvalues of  $\varrho_i$  and  $\tilde{\varrho}_i$ . In fact, the RF expression (8) is applicable to arbitrary two Hermitian and semi-positive definite matrices, which are commuting with each other.

For our model, the RF for the density matrix  $\rho_{ij}$  can be derived explicitly as

$$F_{ij} = \frac{3}{4} \sqrt{(1 + c_{ij}(\lambda))(1 + c_{ij}(\lambda + \delta))} + \frac{1}{4} \sqrt{(1 - 3c_{ij}(\lambda))(1 - 3c_{ij}(\lambda + \delta))}. \quad (9)$$

We see that  $F_{ij}$  depends only on the spin correlator  $c_{ij}$  itself. Therefore, the nontrivial behavior of  $F_{ij}$  is totally determined by that of the corresponding spin correlator. To ensure that the eigenvalues of  $\varrho_1$  and  $\varrho_2$  are non-negative, it is required that  $c_{ij} \in (-1, \frac{1}{3})$ , which subsequently guarantees  $F_{ij} \in [0, 1]$ .

The relation between the RF (9) and QPTs may be understood as follows. The spin correlator  $c_{ij}$  contains all the information of the reduced density matrix  $\rho_{ij}$ , as shown in equations (5)–(7). This indicates that the discontinuity of  $F_{ij}$  roots in that of the elements of  $\rho_{ij}$ . Meanwhile, it is illustrated in [49] that, under some general conditions, the discontinuity of the elements of the reduced density matrix  $\rho_{ij}$  is the origin of that of the first derivative of the GS energy ( $\partial_\lambda E_0$ ), which is another effective measure of first-order QPTs. This means that the discontinuity of the RF and the first derivative of GS energy have the same origins. Thus they are equivalent effective in characterizing first-order QPTs, which is similar to the relation between the global fidelity and first derivative of GS energy [5]. The above analyses are also available for the low-lying ESs, since  $\rho_{ij}$  and  $E_0$  are obtained under the same eigenstate of the Hamiltonian.

### 2.3. Energy spectra

The final result (9) suggests that our task is to calculate the spin correlator  $c_{ij} = \text{tr}(\rho_{ij}\sigma_{iz}\sigma_{jz})$ , where  $\rho_{ij}$  is obtained by tracing out all other spin degrees of freedom except for  $i$  and  $j$ , i.e.,  $\rho_{ij} = \text{tr}_{\bar{ij}}(\rho)$  with  $\rho$  the corresponding global density matrix. In the following, we will concentrate on the RFs for the GS and the low-lying ESs. As we know, for a nondegenerate pure state  $|\Psi_n\rangle$ , the density matrix of the global system can be expressed as  $\rho_n = |\Psi_n\rangle\langle\Psi_n|$ . However, when  $|\Psi_n\rangle$  is degenerate, it is a little trouble to obtain the corresponding density matrix. Thus it is necessary to examine the energy spectra of the Hamiltonian to see the energy degeneracy first.

In figure 1, we explicitly show the low-lying energy spectra of the frustrated Heisenberg chain in the antiferromagnetic case for the system sizes  $N = 6, 8, 10$  and  $N = 7, 9, 11$ . They are mainly divided into two types with even and odd sizes, respectively. For even-size system, the GS is nondegenerate except for the crossing points. However, the first ES for the even-size system is threefold degenerate when  $0 < \lambda < \lambda_{2c}$  ( $\lambda_{2c} \simeq 0.241$ ), and is nondegenerate when  $\lambda > \lambda_{2c}$  except for the crossing points. It is noted that the first ES crosses with both the GS at  $\lambda_{1c} = 0.5$  and the second ES at  $\lambda_{2c} \simeq 0.241$ . Thus it is expected that the RF of the first ES would indicate both the two QPT points as the parameter  $\lambda$  changes. For the odd-size system, the GS is fourfold degenerate except for the crossing points, while the degeneracies of the low-lying ESs become very complex as  $\lambda$  varies. However, it is found excitedly that there still exists a crossing point at which the second and third ESs cross with each other. As  $N$  increases from 7 to 11, this point changes from  $\lambda = 0.281$  to  $\lambda = 0.254$ , which approaches the QPT point  $\lambda_{2c} \simeq 0.241$ . This implies that the RF of the second ES would also exhibit the QPT point  $\lambda_{2c}$  for the odd-size systems.

The degeneracy properties of the above energy spectra can be explained as follows. For the even-size system, according to the Lieb–Mattis theorem [51], the GS of the system in the antiferromagnetic case should be included in the subspace with  $S_z = 0$ , which corresponds to a situation with an equal number of down and up spins. In this subspace, all the spin operators  $S_\alpha$  ( $\alpha = x, y, z$ ) commute with each other, as well as the Hamiltonian  $H$ , thus the GS of the system is nondegenerate except for energy-level crossings [34, 35]. For the odd-size system, the lowest energy of the system exists in the subspaces with  $S_z = \pm 1/2$ . These two subspaces have the same energy spectra due to the  $Z_2$  symmetry of the system, i.e.,  $[H, \bigotimes_i \sigma_{ix}] = 0$ . And in each of these subspaces, the spin operators  $S_\alpha$  do not commute with each other, which

can also induce degeneracy of the GS. Therefore, the GS for the odd-size system is at least fourfold degenerate.

In addition, the real QPT points only exist in the thermodynamic limit, i.e.,  $N \rightarrow \infty$ , which can be treated as an even number. This is why the energy-level crossings of the even-size systems converge more quickly than the odd-size systems to the real QPTs as  $N$  increases. As pointed in [34, 35] that for the odd-size system, as  $N \rightarrow \infty$ , the energy per spin only differs by terms of  $O(1/N)$  compared to the even-size system.

One approach to overcome the above subtle problem induced by the degeneracy is to assume the mixed state as an equal mixture of the degenerate states [31]

$$\rho_n = \frac{1}{D} \sum_{d=1}^D |\Psi_{nd}\rangle \langle \Psi_{nd}|, \tag{10}$$

with  $D$  the degeneracy of the energy  $E_n$  and  $|\Psi_{nd}\rangle$  the  $d$ th degenerate eigenstate of the system. This assumption is not unreasonable when we consider a general mixed state in the thermal equilibrium  $\rho = \exp(-H/T)/Z$  with  $Z = \text{tr}\{\exp(-H/T)\}$  the partition function. If  $\rho_n$  is degenerate, each of its degenerate states has the same probability  $P_{nd} = \exp(-E_n/T)/Z$ , i.e., the degenerate state  $|\Psi_{nd}\rangle$  has an equal mixture weight in the mixed state  $\rho_n$ . In the following, we will adopt this approach to calculate the RF of the system.

### 3. Quantum phase transitions

#### 3.1. Analytical results for $N = 6$ case

For the case that the total spins  $N = 6$ , the GS energy can be analytically obtained in the invariant subspace with  $S_z = 0$ . With the help of the translation symmetry of the system (see [52]), the GS energy is given by [53]

$$E_0 = \begin{cases} -\frac{3}{2}(1 + \lambda), & \lambda \geq 0.5, \\ -\frac{1}{2}(2 + \sqrt{13 - 18\lambda + 9\lambda^2}), & \lambda \leq 0.5, \end{cases} \tag{11}$$

with the corresponding GS

$$|\Psi_0\rangle = \begin{cases} \frac{1}{\sqrt{2}}(|t_1^+\rangle - |t_2^+\rangle), & \lambda \geq 0.5, \\ \frac{1}{\sqrt{\alpha^2 + \beta^2 + 2}}(|t_1^-\rangle - |t_2^-\rangle + \alpha|t_3\rangle + \beta|t_4\rangle), & \lambda \leq 0.5, \end{cases} \tag{12}$$

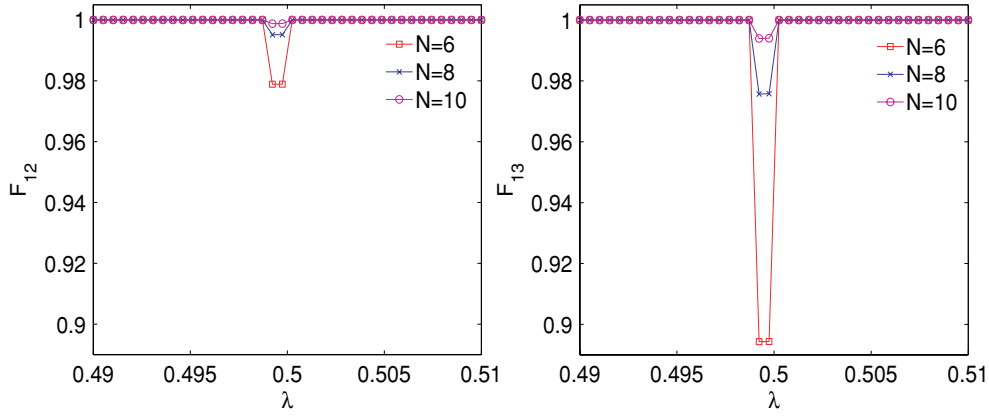
where

$$\begin{aligned} |t_1^\pm\rangle &= \sum_{n=0}^5 (\pm 1)^n T^n |110100\rangle, & |t_2^\pm\rangle &= \sum_{n=0}^5 (\pm 1)^n T^n |001011\rangle, \\ |t_3\rangle &= \sum_{n=0}^5 (-1)^n T^n |000111\rangle, & |t_4\rangle &= \sum_{n=0}^1 (-1)^n T^n |010101\rangle, \end{aligned}$$

with

$$\alpha = \frac{1 - 2\lambda}{3 - \lambda + \sqrt{13 - 18\lambda + 9\lambda^2}}, \quad \beta = -\frac{1}{\sqrt{3}}(\alpha + 2),$$

and  $T$  is the translation operator, i.e.,  $T|0\rangle_i = |0\rangle_{i+1}$  and  $T|1\rangle_i = |1\rangle_{i+1}$ . One can easily check that the GSs for  $\lambda \geq 0.5$  and  $\lambda \leq 0.5$  are orthogonal to each other. Hence, for the global



**Figure 2.** Reduced fidelities  $F_{12}$  (left) and  $F_{13}$  (right) for the ground state versus  $\lambda$  for  $N = 6, 8, 10$  with  $\delta = 10^{-3}$ .

system, the GS fidelity on both sides of  $\lambda = 0.5$  equals to unity, and at the crossing point it drops to zero, see more in [32]. However, for the subsystem, the reduced density matrix only contains partial information of the global one. Thus, the orthogonality of the states on both sides of the crossing point is destroyed and the RF only drops to a finite value.

Then the GS spin correlators of the reduced density matrices  $\rho_{12}$  and  $\rho_{13}$  can be derived from equation (12) as

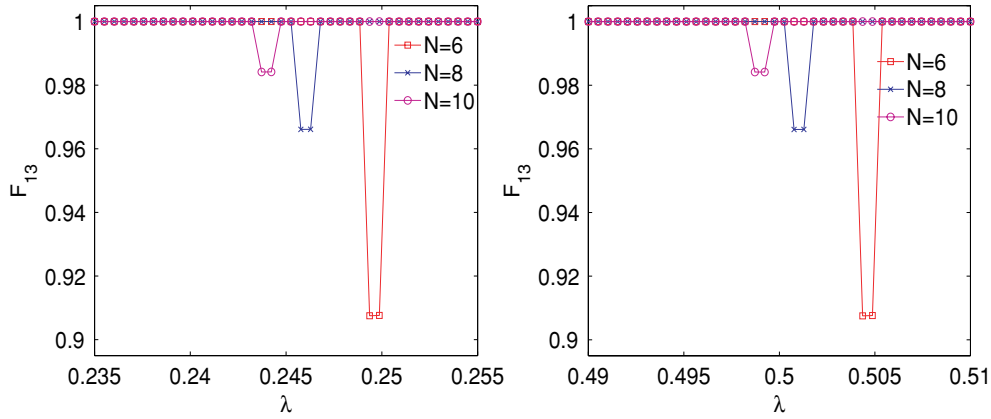
$$\begin{aligned}
 c_{12} &= \begin{cases} \frac{-13+9\lambda-2\sqrt{13-18\lambda+9\lambda^2}}{9\sqrt{13-18\lambda+9\lambda^2}}, & \lambda < 0.5, \\ -\frac{7}{15}, & \lambda = 0.5, \\ -\frac{1}{3}, & \lambda > 0.5, \end{cases} \\
 c_{13} &= \begin{cases} \frac{1-\lambda}{\sqrt{13-18\lambda+9\lambda^2}}, & \lambda < 0.5, \\ -\frac{1}{15}, & \lambda = 0.5, \\ -\frac{1}{3}, & \lambda > 0.5. \end{cases}
 \end{aligned} \tag{13}$$

The above results at the point  $\lambda = 0.5$  is obtained by using the approach shown in equation (10). Then substitute equation (13) into equation (9), we obtain the final expressions of the fidelities  $F_{12}$  and  $F_{13}$ . Since the spin correlators  $c_{12}$  and  $c_{13}$  are discontinuous at  $\lambda = 0.5$ , so do the fidelities  $F_{12}$  and  $F_{13}$ , as shown in figure 2. In addition, equation (13) shows that when  $\lambda \rightarrow (0.5)^-$ ,  $c_{12} \rightarrow -3/5$  and  $c_{13} \rightarrow 1/5$ , and when  $\lambda \rightarrow (0.5)^+$ ,  $c_{12}, c_{13} \rightarrow 1/3$ . That is, the difference between the left limit and the right limit of  $c_{13}$  is greater than that of  $c_{12}$ . It means the spin correlator is more sensitive at the QPT point for long-range spin coupling. This leads to the result that  $F_{13}$  is more singular than  $F_{12}$  in the vicinity of QPT points, which is compared precisely in figure 2.

### 3.2. Numerical results for $N = 6, 8, 10$

In general, it is not an easy work to get the analytical results for  $N > 6$ , thus we have to appeal to the numerical method, i.e., exact diagonalization. In the following, the results are shown in the even- and odd-size systems, respectively.



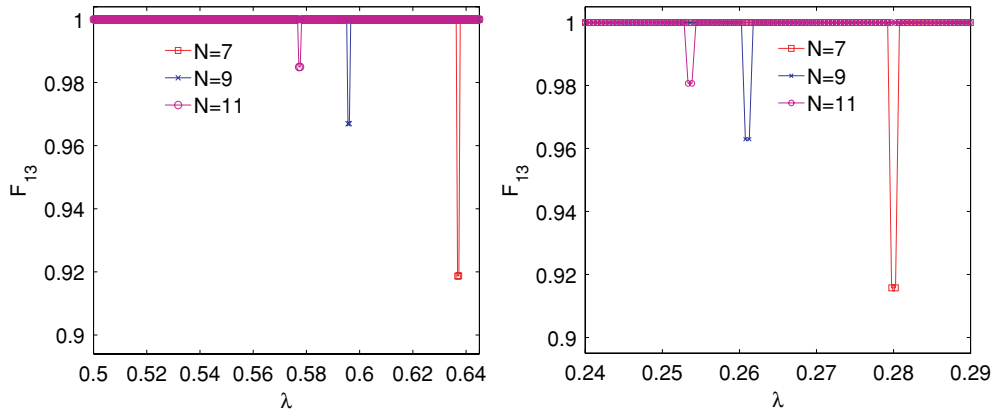


**Figure 3.** Reduced fidelities  $F_{13}$  for the first-excited state around two different QPT points, i.e.,  $\lambda_{2c} = 0.241$  (left) and  $\lambda_{1c} = 0.5$  (right), versus  $\lambda$  for  $N = 6, 8, 10$  with  $\delta = 10^{-3}$ .

In figure 2, we plot the RFs  $F_{12}$  and  $F_{13}$  for the GS versus the parameter  $\lambda$  for different system sizes  $N = 6, 8, 10$ . First, we see that both  $F_{12}$  and  $F_{13}$  become discontinuous at the first-order QPT point  $\lambda_{1c} = 0.5$ . As the system size increases, the discontinuous behavior around  $\lambda_{1c} = 0.5$  becomes more and more weak. It may be explained as follows. The relation between RF ( $F_R$ ) and global fidelity ( $F_G$ ) satisfies  $F_R \geq F_G$  [54]. For the QPTs associated with energy-level crossing, the discontinuity of global fidelity at the QPT points results from the orthogonality of the states on the two sides of the point. At this point, there is a sudden drop of  $F_G$  from 1 to 0. Then for a small subsystem, the orthogonality may be destroyed. As the system size increases, it becomes more and more weak for the subsystem to reflect the global information of the system. In the thermodynamic limit, the orthogonality may be destroyed completely, and there is almost no drop of the RF at the QPT points. In this case,  $F_R \rightarrow 1$  at the QPT points, and it may not effectively exhibit the QPTs. In contrast, the previous works [15, 17–20] show that, for the QPTs connected to avoided level crossings, the information of the subsystem may still reflect the dramatic change of the global structure. With the increasing of  $N$ , the RF becomes more and more singular around the QPT points. Moreover, we found that [18] the reduced fidelity susceptibility takes on a similar scaling behavior as the global one. The distinctness of the RF in characterizing these two types of QPTs might be very interesting, and further deep discussion is needed. In conclusion, for our system, the RF can only reflect the nontrivial behavior of the finite-size systems at the QPT points. However, this seems enough for usual calculation requirement.

Then comparing the two RFs for a given system size, we find that  $F_{13}$  is obviously more sensitive than  $F_{12}$  around the QPT point. This may be because the subsystem with long-range spin coupling contains more information of the whole system, as analyzed in section 3.1. Thus in the following, our calculations are concentrated on the RF between the NNN spins.

As it is illustrated in section 2.1 that there is another QPT point at about  $\lambda_{2c} \simeq 0.241$ , which corresponds to the first and second-excited energy-level crossing for the even-size system. In [32], they have used the fidelity of the first ES as an indicator of this point. Here we would like to apply the RF approach to detect it, which is shown in the left-hand figure of figure 3. It is seen that the discontinuous point of  $F_{13}$  approaches 0.241 with the system size increasing, even though the nontrivial behavior becomes weaker. This again proves that the



**Figure 4.** Reduced fidelities  $F_{13}$  for the ground state (left) and the second-excited state (right) versus  $\lambda$  for  $N = 7, 9, 11$  with  $\delta = 10^{-3}$ .

fidelity of the first ES might be a good indicator of the BKT QPTs, no matter it is for the global or reduced system. Meanwhile, as shown in the right-hand figure of figure 3, the fidelity of the first ES can also be used to detect the first-order QPT point  $\lambda_{1c}$ . In this sense, the fidelity of first ES is an effective indicator for both the first-order and the BKT QPTs.

### 3.3. Numerical results for $N = 7, 9, 11$

The different energy structures between the odd-size and even-size systems result in the difference between the singular behavior of the respective RFs. In figure 4, the RFs  $F_{13}$  for the GS and the second ES versus the parameter  $\lambda$  are displayed. As it is expected that the RF for the GS can also exhibit the nontrivial behavior around  $\lambda_{1c} = 0.5$ . With the increasing system size, the discontinuous point of  $F_{13}$  approaches  $\lambda_{1c}$  quickly. Moreover, compared to  $F_{13}$  for the GS of the even-size system as shown in the right-hand figure of figure 2, the discontinuous behavior of RF in the odd-size system disappears a little slower. This means for the odd-size system, the information of the global system stored in the subsystem losses slower as the system size increases. From the right-hand figure of figure 4, we see that the RF  $F_{13}$  for the second ES also well reflects the nontrivial behavior of the finite-size system around  $\lambda_{2c} \simeq 0.241$ . This further testifies the fact that the fidelity of the low-lying ESs is a good indicator of the QPTs of the system.

## 4. Conclusion

In conclusion, in terms of RF, we have studied the nontrivial behavior of the 1D spin-1/2 antiferromagnetic Heisenberg chain with frustration around the QPT points of the system. It is shown that the RF of this system is totally determined by the corresponding spin correlator. We examine the energy structure for the finite-size systems, and find there are some differences between the energy structures with even and odd sizes, which leads to the different behavior of RFs of the two kinds of systems. We calculate the RFs between NN and NNN spin pairs both for the GS and the low-lying ESs in the finite-size systems. We find the RF between NNN spins is more sensitive at the QPT points than the NN case, and the RF of the low-lying ES is also a good indicator for QPTs of the system.

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