

Reduced-fidelity approach for quantum phase transitions in spin- $\frac{1}{2}$ dimerized Heisenberg chains

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We show a general connection between the reduced-fidelity susceptibility and quantum phase transitions, and derive an explicit expression of the reduced-fidelity susceptibility for the one-dimensional spin-1/2 dimerized Heisenberg chain, which has both SU(2) and translational symmetries. We find that the reduced-fidelity susceptibility is directly related to the square of the second derivative of ground-state energy, which means that it is an effective indicator of the second-order quantum phase transitions. In terms of this indicator, we explicitly examine the critical behavior of the spin-1/2 dimerized Heisenberg chain. Moreover, we give another two exemplifications to show that the results may also be extended to high-spin systems.

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I. INTRODUCTION

Quantum phase transitions (QPTs) is an essential phenomenon in quantum many-body correlated system. It was induced by the ground-state (GS) transition driven by external parameters at zero temperature. The question of how to characterize QPTs has attracted widespread attention. Conventionally, QPTs are described in terms of order parameter and symmetry breaking within the Landau-Ginzburg paradigm.¹ One object in these traditional ways is that there is no general method to find the order parameter for a common system. To overcome this problem, a concept called *fidelity*^{2,3} [see Eqs. (2) and (3)] was borrowed from the field of quantum-information theory since it well describes the overlap between two states in different phases with different structural properties. Thus it does not need *a priori* knowledge of the order parameter in detecting QPTs. On the other hand, *fidelity susceptibility*^{4,5} [see Eq. (4)] was found to be more convenient than fidelity itself for its independence of the slightly changed external parameters. Hitherto, these two connected concepts have succeeded in identifying the QPTs of many systems, such as XY spin chain,³ XXZ chain,⁶ Hubbard model,^{7,8} frustrated Heisenberg chain,⁹ Kitaev honeycomb model,¹⁰ and extended Harper model.¹¹ The intrinsic relation between the GS fidelity (or fidelity susceptibility) and the characterization of a quantum phase transition has been studied in Ref. 12. It was shown that the singularity and scaling behavior of the GS fidelity (or fidelity susceptibility) are directly related to its corresponding derivative of GS energy, which characterizes the QPTs conventionally. Moreover, the fidelity susceptibility is associated with dynamic structure factor for QPTs, and with specific heat and magnetic susceptibilities for thermal phase transitions.¹³

The above works are all concerned with the global GS fidelity. Then there is a natural question of whether the fidelity of the subsystem, i.e., the *reduced fidelity* (or named *partial-state fidelity*) could reflect the QPTs. Recently, some works have been devoted to this subject. Zhou *et al.*¹⁴ found that it succeeds in capturing nontrivial information along renormalization group flows and in detecting the QPTs in XY model.¹⁵ Paunković *et al.*¹⁶ showed that it enables them to identify the on-site magnetization as the order parameter for

the phase transition in the conventional BCS superconductor with an inserted magnetic impurity system. Kwok *et al.*¹⁷ tested its effectiveness in characterizing the QPTs of the isotropic Lipkin-Meshkov-Glick model and the antiferromagnetic one-dimensional (1D) Heisenberg model. Meanwhile, we derived a general expression for the two-site reduced-fidelity susceptibility (RFS). It has been applied to the study of the Lipkin-Meshkov-Glick model¹⁸ and transverse field Ising model.¹⁹ We found that the RFS shows similar scaling behavior to the global fidelity susceptibility. All the above works illustrate that the reduced-fidelity approach is also an effective tool in identifying QPTs. However, a general relation between RFS and QPTs is not established. In this work, we will illustrate the general relation between RFS and QPTs in terms of the reduced density matrix (RDM), and build an explicit connection between the RFS and the second-order QPTs for the spin-1/2 dimerized Heisenberg chain based on its SU(2) and translational symmetries.

The dimerized Heisenberg chain is a fundamental spin-correlated model. It is of special interest both in theory and experiment since it gives a reasonably accurate description of many quasi-one-dimensional (quasi-1D) antiferromagnets which have two important but structurally inequivalent superexchange paths that are spatially linked, such as the materials of Cu(NO₃)₂·2.5H₂O, (VO)₂P₂O₇, and various aromatic free-radical compounds.²⁰ Therefore, many efforts have been devoted to study its quantum critical behavior of the dimerized Heisenberg model using various methods, e.g., continuous unitary transformations,²¹ density-matrix renormalization group,²² concurrence,²³ and block entanglement.²⁴ Here we employ the reduced-fidelity approach to study the QPTs of this model. The Hamiltonian for the spin-1/2 dimerized Heisenberg chain reads

$$H_D = \sum_{i=1}^{N/2} (\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + \alpha \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}), \quad (1)$$

where \mathbf{S}_i denotes the i th spin-1/2 operator, and α is the ratio between the two kinds of nearest-neighbor (NN) couplings. The total number of spins N is required to be even and the periodic boundary condition $\mathbf{S}_1 = \mathbf{S}_{N+1}$ is assumed. Obviously, this Hamiltonian has both SU(2) and translational

symmetries, which lead to an interesting relation between RFS and QPTs shown in Eq. (18).

This paper is organized as follows. In Sec. II, we show the general connection between RFS and QPTs in terms of RDM, and derive an expression of RFS for spin-1/2 systems with SU(2) symmetry, then apply it to the spin-1/2 dimerized Heisenberg chain, whose translational symmetry further enables us to get a direct relation between RFS and the second derivative of GS energy. In Sec. III, the critical behavior of the spin-1/2 dimerized Heisenberg chain is carefully discussed for both finite-size and infinite-size situations. In Sec. IV, further extension of the results in spin-1/2 case to high-spin case is enumerated by two other exemplifications. Finally, a summary is presented in Sec. V.

II. REDUCED-FIDELITY SUSCEPTIBILITY AND ITS CONNECTION TO QUANTUM PHASE TRANSITIONS

In this section, we will discuss the relation between RFS and QPTs. First, we briefly review the definitions of fidelity and fidelity susceptibility. For two pure states $|\Psi(\alpha)\rangle$ and $|\Psi(\alpha+\delta)\rangle$ with δ as a small change in the external parameter α , their overlap or *fidelity* is defined as³

$$F(\alpha) = |\langle \Psi(\alpha) | \Psi(\alpha + \delta) \rangle|. \quad (2)$$

The extension to the mixed states is in general the *Uhlmann fidelity*^{25,26}

$$F(\alpha) = \text{tr} \sqrt{\rho(\alpha)^{1/2} \rho(\alpha + \delta) \rho(\alpha)^{1/2}}, \quad (3)$$

with $\rho(\alpha)$ and $\rho(\alpha + \delta)$ as the two density matrices. The fidelity susceptibility is defined as

$$\chi = \lim_{\delta \rightarrow 0} \frac{-2 \ln F}{\delta^2}, \quad (4)$$

which does not depend on δ . For a RDM, it is always a mixed state. Thus it is convenient to define the corresponding reduced fidelity in terms of Uhlmann fidelity (3). Accordingly, the RFS can be described as Eq. (4).

A. General connection between RFS and QPTs

Then we will show the general relation between RFS and QPTs. It is noticed that the definition of RF (3) depends only on the RDM, which may contain sufficient information about QPTs. This inspires us to infer that, for a more general case, QPTs are essentially related to the RDM. In Ref. 27, they have provided a powerful substantiation. They demonstrated that, under certain general conditions, the elements of two-body RDM are able to signal the QPTs. They consider a general Hamiltonian that contains two-body interaction such as

$$H = \sum_{i\alpha\beta} \epsilon_{\alpha\beta}^i |\alpha_i\rangle\langle\beta_i| + \sum_{ij\alpha\beta\gamma\kappa} V_{\alpha\beta\gamma\kappa}^{ij} |\alpha_i\rangle|\beta_j\rangle\langle\gamma_i|\langle\kappa_j|, \quad (5)$$

where i and j enumerate N particles, and $\{|\alpha_i\rangle\}$ is a basis for the Hilbert space. For the nondegenerate GS $|\psi\rangle$, its GS energy is $E_0 = \langle \psi | H | \psi \rangle$, and the element of the corresponding two-particle RDM is $\rho_{\gamma\delta\alpha\beta}^{ij} = \langle \psi | \alpha_i \beta_j \rangle \langle \gamma_i \kappa_j | \psi \rangle$. Thus the rela-

tion between energy and RDM is $E_0 = \sum_{ij} \text{tr}[U(ij)\rho^{ij}]$, where $U_{\alpha\beta\gamma\kappa}(ij) = \epsilon_{\alpha\gamma}^i \delta_{\beta\kappa}^j / N_i + V_{\alpha\beta\gamma\kappa}^{ij}$ with N_i as the number of particles that particle i interacts with and $\delta_{\beta\kappa}^j$ as the Kronecker symbols on particle j . Then using the Feynman-Hellman theorem,²⁸ i.e., $\partial_\xi E_n = \langle n | \partial_\xi H | n \rangle$ with $|n\rangle$ as the nondegenerate eigenstate of Hamiltonian H and E_n as the eigenenergy, the derivatives of energy per particle ($e_0 \equiv E_0/N$) are obtained as

$$\partial_\xi e_0 = \frac{1}{N} \sum_{ij} \text{tr}\{[\partial_\xi U(ij)]\rho_{ij}\}, \quad (6)$$

$$\partial_\xi^2 e_0 = \frac{1}{N} \sum_{ij} \{\text{tr}\{[\partial_\xi^2 U(ij)]\rho_{ij}\} + \text{tr}\{[\partial_\xi U(ij)]\partial_\xi \rho_{ij}\}\}, \quad (7)$$

where it follows from Eq. (6) that $\sum_{ij} \text{tr}[U(ij)(\partial_\xi \rho_{ij})] = 0$. As is known, according to the classical definition of phase transitions given in terms of the free energy,²⁹ in the limit of $T=0$, a first-order QPT (second-order QPT) is characterized by a discontinuity in the first (second) derivative of the GS energy [see also Eq. (19)]. Therefore, if $U(ij)$ is a smooth function of the Hamiltonian parameter ξ , the origin of first-order QPTs is due to the discontinuity of one or more of the ρ_{ij} 's at the critical point according to Eq. (6). Whereas, if ρ_{ij} is finite at the critical point, the origin of second-order QPTs is the fact that one or more of the $\partial_\alpha \rho_{ij}$'s diverge at the critical point.

Based on these facts, one finds that if $U(ij)$ is a smooth function and the first derivative of the elements of ρ_{ij} diverges at the critical point, then $\partial_\xi^2 e_0$ diverges as well, which indicates a second-order QPT. Thus the relation revealed by Eq. (7) may be the origin of the relation between RFS and QPTs. This is not restricted to the systems with certain symmetry, and a more explicit and direct relation between RFS and QPTs may need further deep considerations.

In addition, the relation between the reduced fidelity (denoted as F_R) and its corresponding global fidelity F_G is given already as $F_G \leq F_R$.³⁰ According to relation (4), the corresponding susceptibilities satisfy $\chi_G \geq \chi_R$. However, all the previous works¹⁴⁻¹⁹ and this work confirm that the reduced fidelity is as effective as global fidelity in characterizing QPTs, and in some cases, such as the models mentioned below, it is only necessary to know the GS energy of system in calculating the RFS rather than its GS for the global fidelity, which is generally not easy to be obtained.

B. RFS for spin-1/2 systems with SU(2) symmetry

To show an explicit relation between RFS and QPTs, we would like to consider a class of spin-1/2 systems with SU(2) symmetry. The SU(2) symmetry, i.e., $[H, \sum_{i=1}^N S_{i\gamma}] = 0$ ($\gamma = x, y, z$), guarantees that the RDM between two NN spins is of the form³¹

$$\rho_{ij} = \text{diag}(\varrho_1, \varrho_2), \quad (8)$$

with

$$\varrho_1 = \begin{pmatrix} u^+ & 0 \\ 0 & u^+ \end{pmatrix}, \quad \varrho_2 = \begin{pmatrix} u^- & w \\ w & u^- \end{pmatrix}, \quad (9)$$

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 by³¹

$$u^\pm = \frac{1}{4}(1 \pm \langle \sigma_{iz} \sigma_{jz} \rangle),$$

$$w = \frac{1}{2} \langle \sigma_{iz} \sigma_{jz} \rangle. \quad (10)$$

This implies that the RDM ρ_{ij} is only related to the spin correlator $\langle \sigma_{iz} \sigma_{jz} \rangle$. It is noticed that both ϱ_1 and ϱ_2 are Hermitian, and they can be rewritten in terms of Pauli operators as $\varrho_1 = u^+ \mathbf{I}$ and $\varrho_2 = u^- \mathbf{I} + w \sigma_x$, where \mathbf{I} denotes a 2×2 identity matrix. Therefore, it is found that $\varrho_i \equiv \varrho_i(\alpha)$ ($i=1, 2$) commutes with $\tilde{\varrho}_i \equiv \varrho_i(\alpha + \delta)$, with δ as a small perturbation of the control parameter α , i.e., $[\varrho_i, \tilde{\varrho}_i] = 0$. This commuting property will greatly facilitate our study of RFS below.

With the definition of fidelity, we get

$$F_{\varrho_k} = \text{tr} \sqrt{\varrho_k^{1/2} \tilde{\varrho}_k \varrho_k^{1/2}} = \sum_l \sqrt{\lambda_l \tilde{\lambda}_l}, \quad (11)$$

where λ_l and $\tilde{\lambda}_l$ are the eigenvalues of ϱ_k and $\tilde{\varrho}_k$, respectively. Since zero eigenvalues have no contribution to F_{ϱ_k} , we only need to consider the nonzero ones. In the following, the subscript l in Σ_l only refers to the nonzero eigenvalues of ϱ_k . For a small change δ , $\tilde{\lambda}_l$ can be expanded as $\tilde{\lambda}_l \equiv \lambda_l(\alpha + \delta) \simeq \lambda_l + (\partial_\alpha \lambda_l) \delta + (\partial_\alpha^2 \lambda_l) \delta^2 / 2 + O(\delta^3)$. Then the fidelity for matrix ϱ_l becomes

$$F_{\varrho_k} = \sum_l \left\{ \lambda_l + \frac{\delta}{2} \partial_\alpha \lambda_l + \frac{\delta^2}{4} \left(\partial_\alpha^2 \lambda_l - \frac{(\partial_\alpha \lambda_l)^2}{2\lambda_l} \right) \right\}. \quad (12)$$

Here we have neglected small terms higher than second order. Since $\Sigma_l \lambda_l \equiv 1$, we have $\Sigma_l \partial_\alpha \lambda_l = \Sigma_l \partial_\alpha^2 \lambda_l = 0$. Thus the fidelity is further reduced to

$$F_{\varrho_k} = 1 - \frac{\delta^2}{2} \sum_l \frac{(\partial_\alpha \lambda_l)^2}{4\lambda_l}. \quad (13)$$

Therefore, according to the relation between fidelity and susceptibility, $F = 1 - \chi \delta^2 / 2$, which is equivalent to Eq. (4), the fidelity susceptibility χ_{ϱ_k} corresponding to the matrix ϱ_k is obtained as

$$\chi_{\varrho_k} = \sum_l \frac{(\partial_\alpha \lambda_l)^2}{4\lambda_l}. \quad (14)$$

This expression of fidelity susceptibility is valid for any commuting density matrices, and the second power on the right-hand side of the equation will lead to an interesting relation between the RFS and the second derivative of GS energy shown in Eq. (18).

By using the expression of the RDM [see Eqs. (8)–(10)], after some calculations, the RFS for the density matrix ρ_{ij} is derived as

$$\chi_{ij} = \chi_{\varrho_1} + \chi_{\varrho_2} = \frac{4(\partial_\alpha \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)^2}{(3 + 4\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)(1 - 4\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle)}$$

$$= \frac{3(\partial_\alpha \langle \sigma_{iz} \sigma_{jz} \rangle)^2}{4(1 + \langle \sigma_{iz} \sigma_{jz} \rangle)(1 - 3\langle \sigma_{iz} \sigma_{jz} \rangle)}, \quad (15)$$

which depends on both the spin correlator $\langle \sigma_{iz} \sigma_{jz} \rangle$ itself and its first derivative. In fact, to ensure that the eigenvalues of ϱ_1 and ϱ_2 are positive (we do not consider the zero eigenvalues), it is required

$$\langle \sigma_{iz} \sigma_{jz} \rangle \in \left(-1, \frac{1}{3} \right), \quad (16)$$

which subsequently guarantees the susceptibility is non-negative.

C. RFS for spin-1/2 dimerized Heisenberg chain

Furthermore, we apply the above results to the spin-1/2 dimerized Heisenberg chain, whose Hamiltonian is shown in Eq. (1). We will see that the translational symmetry of this system will result in an interesting result.

The translational symmetry of the Hamiltonian leads to the fact that any two terms of the form $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ is equal to each other. Applying the Feynman-Hellman theorem²⁸ to the GS of the system, the spin correlators corresponding to two NN spin pairs are written as

$$\langle \sigma_{1z} \sigma_{2z} \rangle = \frac{8}{3}(e_0 - \alpha \partial_\alpha e_0),$$

$$\langle \sigma_{2z} \sigma_{3z} \rangle = \frac{8}{3} \partial_\alpha e_0, \quad (17)$$

where $e_0 \equiv E_0/N$ represents the GS energy (denoted by E_0) per spin. Substituting Eq. (17) into Eq. (15), one can get the explicit forms for the RFSs χ_{12} and χ_{23} as follows

$$\chi_{12} = \frac{16\alpha^2 (\partial_\alpha^2 e_0)^2}{(3 + 8e_0 - 8\alpha \partial_\alpha e_0)(1 - 8e_0 + 8\alpha \partial_\alpha e_0)},$$

$$\chi_{23} = \frac{16(\partial_\alpha^2 e_0)^2}{(3 + 8\partial_\alpha e_0)(1 - 8\partial_\alpha e_0)}. \quad (18)$$

One key observation is that the numerators of the above two expressions happen to be proportional to the square of the second derivative of GS energy. Since the first derivative of energy is easily checked to be continuous [see Eq. (24)], and the denominators are ensured to be positive and finite by Eq. (16), the singularities of the RFSs are determined only by the numerators. That is, if the second derivative of GS energy is singular at the critical point, the RFSs are singular as well. On the other hand, it is known that the divergence of the second derivative of GS energy reflects the second-order QPTs of the system, which is shown in Ref. 12 explicitly as

$$\partial_\alpha^2 e_0 = \sum_{n \neq 0} \frac{2|\langle \Psi_n | H_1 | \Psi_0 \rangle|^2}{N(E_0 - E_n)}, \quad (19)$$

where $H_1 = \partial_\alpha H$ is the driving term of the Hamiltonian H , and $|\Psi_n\rangle$ is the eigenvector corresponding to the eigenvalue E_n of

H. Equation (19) shows that the vanishing energy gap in the thermodynamic limit (TL) can lead to the singularity of the second derivative of GS energy. Therefore, both the two-spin RFSs can exactly reflect the second-order QPTs in this model. In addition, the second power in the numerators of the expressions, which originates from the relation obtained in Eq. (14), indicates that the two-spin RFSs is more effective than the second derivative of the GS energy in measuring QPTs. Furthermore, by the fidelity approach, it will be shown in Sec. III that the dimerized antiferromagnetic Heisenberg chain (AHC) has a second-order critical point at $\alpha=1$.

III. CRITICAL BEHAVIOR OF SPIN-1/2 DIMERIZED HEISENBERG CHAIN

In the following, in terms of RFS obtained in Eq. (18), we consider the critical behavior of the 1D spin-1/2 dimerized Heisenberg chain in the antiferromagnetic case. It is known that, for $0 < \alpha \ll 1$, the coupling between two dimers is so weak that all the spins are locked into singlet states, while for $\alpha=1$, the system is reduced to the uniform AHC. Hence, it has already been proven that the dimerized model has a critical point at $\alpha=1$,²¹⁻²⁴ which exactly exists in the thermodynamic limit $N \rightarrow \infty$.

A. Finite-size behavior

1. Analytical results for $N=4$ case

For the case of the total spins $N=4$, the analytical results can be obtained. In this case, the GS energy per spin of the system is^{23,32}

$$e_0 = -\frac{1}{4} \left(\frac{1+\alpha}{2} + \sqrt{1-\alpha+\alpha^2} \right), \quad (20)$$

with its first and second derivatives being

$$\begin{aligned} \partial_\alpha e_0 &= \frac{1}{8} \left(-1 + \frac{1-2\alpha}{\sqrt{1-\alpha+\alpha^2}} \right), \\ \partial_\alpha^2 e_0 &= -\frac{3}{16(1-\alpha+\alpha^2)^{3/2}}. \end{aligned} \quad (21)$$

Then the susceptibilities of the RDMs ρ_{12} and ρ_{23} can be derived from Eq. (18) as

$$\chi_{12} = \chi_{23} = \frac{3}{16(1-\alpha+\alpha^2)^2}. \quad (22)$$

From Eq. (22) we see that χ_{12} and χ_{23} have the same expressions, and there is no singularity over parameter α . However, taking derivation of the expression with respect to α , one will find that there is a maximum of χ_{12} (or χ_{23}) at $\alpha=0.5$, which is also the maximum position of $\partial_\alpha^2 e_0$ as shown in Eq. (21). However, the maximum position $\alpha=0.5$ deviates from the real critical point $\alpha=1$ and can be called *pseudocritical point* due to the finite size of the system. In addition, the different powers in the expressions of χ_{12} (or χ_{23}) and $\partial_\alpha^2 e_0$ over the factor $(1-\alpha+\alpha^2)$, i.e., the former is 3/2 and the

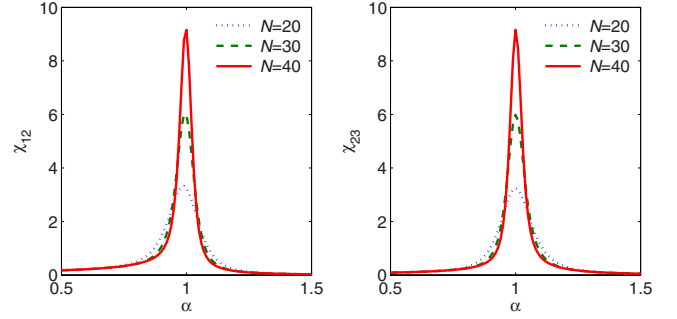


FIG. 1. (Color online) Reduced-fidelity susceptibilities χ_{12} and χ_{23} versus α for $N=20, 30, 40$ of the spin-1/2 dimerized Heisenberg chain.

latter is 2, shows that the RFS is more sensitive around the critical point.

Besides, the exact equivalence between χ_{12} and χ_{23} is in contrast with concurrences as shown in Ref. 23. There, the concurrences for the reduced system, i.e., C_{12} and C_{23} , are unequal to each other and have a crossing point at $\alpha=1$, which leads to the mean concurrence taking its maximum at the critical point $\alpha=1$. This is because the concurrences C_{12} and C_{23} are only related to the GS energy, and its first derivative over α , respectively. However, the RFSs shown in Eq. (18) are also determined by the second derivative of GS energy, which leads to the identical behavior between χ_{12} and χ_{23} .

2. Numerical results

For the case of the total spins $N > 4$, we employ an implementation of the density-matrix renormalization-group method in the ALPS library,³³ and the results are displayed in Fig. 1.

It is seen that both the RFSs χ_{12} and χ_{23} can well reflect the critical behavior of the system. With increasing system size, the pseudocritical point exhibited by χ_{12} (or χ_{23}) approaches to the real critical point $\alpha=1$. Besides, the larger the N becomes, the higher and sharper the peak of χ_{12} (or χ_{23}) is. It should be noticed that there is a slight difference between χ_{12} and χ_{23} for a given α and N , which results from the difference between the spin correlators shown in Eq. (17). Moreover, when N becomes larger, the difference becomes smaller and smaller. In fact, the two-spin correlators are equivalent if we exchange the two kinds of NN couplings. Thus χ_{12} and χ_{23} are also qualitatively equivalent in identifying QPTs.

B. Infinite-size behavior

Now, we consider the critical behavior in the thermodynamic limit. To be consistent with the former works, we adopt a parameter $\eta \equiv (1-\alpha)/(1+\alpha)$. When the system approaches to the uniform chain limit, i.e., $\eta \rightarrow 0$, analytical studies obtained by renormalization group^{34,35} had predicted that the GS energy per spin e_0 should diverge as a power law times a logarithmic correction, i.e., $\eta^{4/3}/|\ln \eta|$. However, it is restricted to an extremely small range $\eta < 0.02$.²² Thereafter, some numerical results pointed out that a pure power-law

behavior is reasonably simple and accurate for larger η as well.^{22,36,37}

For generality, we assume a power law of e_0 as the form $c\eta^p$ with c as an overall constant. The exponent p is given differently over different η ranges. Hitherto, almost all the works^{22,36,37} show that $1 < p < 2$ over the range $0 < \eta < 1$. For example, using the density-matrix renormalization-group approach, in Ref. 22 the exponent is fit to be $p=1.45$ over the range of $0.008 \leq \eta \leq 0.1$ with $c=0.39$, and in Ref. 37, it is estimated in the range of $0.001 \leq \eta \leq 0.1$ as that $p=1.4417$ with $c=0.3891$. Thus we will restrict $1 < p < 2$ in the following. The GS energy per spin in the thermodynamic limit can be written accordingly as²²

$$e_0(\eta) = \frac{1}{1+\eta} [e_0(0) - c\eta^p], \quad (23)$$

where $e_0(0)=1/4-\ln 2$ is the GS energy per spin for $\eta=0$.

The above expression shows that the GS energy follows the power-law behavior η^p . This gives a prediction of the

critical point of the RFSs. From Eq. (23), we can easily get the first and second derivatives of GS energy per spin in the thermodynamic limit as

$$\partial_\alpha e_0 = \frac{c}{2}(2p + \alpha - 1)(1 + \alpha)^{-1}(1 - \alpha)^{p-1},$$

$$\partial_\alpha^2 e_0 = -2c(p-1)p(1 + \alpha)^{-(p+1)}(1 - \alpha)^{p-2}. \quad (24)$$

It is seen that, as $\alpha > 0$ and $1 < p < 2$, the first derivative of e_0 does not diverge for any allowed α value while the second derivative of e_0 has a singular point $\alpha=1$. According to Eq. (18), it is no doubt that the RFSs also diverge at $\alpha=1$. That is, the dimerized Heisenberg chain has a second-order critical point $\alpha=1$.

Next we discuss the critical behavior of the RFSs around the critical point. Inserting Eq. (24) into Eq. (18), we obtain the RFSs as

$$\chi_{12} = -\frac{c^2 p^2 (p-1)^2 \eta^{-2+2p} (\eta-1)^2 (\eta+1)^4}{16 [c^2 (p+\eta-p\eta)^2 \eta^{2p} + c(2\ln 2-1)(p+\eta-p\eta)\eta^{1+p} + \ln 2(\ln 2-1)\eta^2]},$$

$$\chi_{23} = -\frac{c^2 p^2 (p-1)^2 \eta^{-2+2p} (\eta+1)^6}{16 [c^2 (p-\eta+p\eta)^2 \eta^{2p} - c(2\ln 2-1)(p-\eta+p\eta)\eta^{1+p} + \ln 2(\ln 2-1)\eta^2]}. \quad (25)$$

When $\alpha \rightarrow 1$, i.e., $\eta \rightarrow 0$, we only consider the leading terms in the expressions and get the critical behavior of the RFSs as

$$\chi_{12}, \chi_{23} \sim \eta^{2p-4} \sim (1-\alpha)^{2p-4}. \quad (26)$$

Obviously, for $1 < p < 2$, both of them diverge at $\eta=0$, i.e., $\alpha=1$, as displayed in Fig. 2. It is shown that the two RFSs diverge quickly when α approaches one. For a given α , χ_{12} and χ_{23} are remarkably larger than those in the finite-size

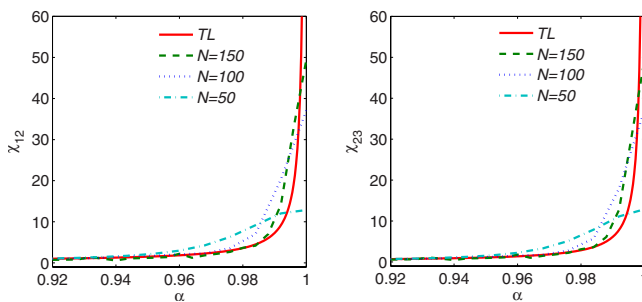


FIG. 2. (Color online) Reduced-fidelity susceptibilities versus α for $N=50, 100, 150$, and in the TL of the spin-1/2 dimerized Heisenberg chain. In the thermodynamic limit, the parameters are given as: $c=0.3891$ and the exponent $p=1.4417$ over the range of $0.001 \leq \eta \leq 0.1$ (Ref. 37), i.e., $0.8182 \leq \alpha \leq 0.9880$.

cases. The different powers between $\partial_\alpha^2 e_0$ and $\chi_{12}(\chi_{23})$ over the factor $(1-\alpha)$ indicate that these RFSs are more singular around the critical point. In addition, with the increasing of the system sizes, i.e., $N=50 \rightarrow 150$, the behavior of $\chi_{12}(\chi_{23})$ approaches that in the thermodynamic limit, which convinces us of the validity of the RFS in the thermodynamic limit as shown in Eq. (25).

IV. EXTENSIONS TO HIGH-SPIN SYSTEMS

In the above, we have explicitly illustrated the connection between RFS and QPTs in the spin-1/2 dimerized Heisenberg chain, which has both SU(2) and translational symmetries. Actually, the results shown in Eq. (18) can also be extended to some high-spin systems possessing the two symmetries. In the following, we would like to briefly give two further exemplifications. One is the mixed-spin (1/2, S) dimerized Heisenberg chain with S as an arbitrary spin length, the other is the spin-1 bilinear-biquadratic model.

The Hamiltonian for the mixed-spin dimerized Heisenberg chain with alternated spins \mathbf{S}_1 and \mathbf{S}_2 is

$$H_F = \sum_{i=1}^{N/2} (\mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} + \alpha \mathbf{S}_{2,i} \cdot \mathbf{S}_{1,i+1}), \quad (27)$$

where \mathbf{S}_1 and \mathbf{S}_2 denote the spin-1/2 and spin- S operators, respectively, and α is the ratio between the two kinds of NN

spin couplings. The periodic boundary condition is assumed. The RFS of the system has been obtained as³⁸

$$\chi_{ij} = \frac{(\partial_\alpha \langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)^2}{(S - 2\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)(S + 1 + 2\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,j} \rangle)}. \quad (28)$$

Meanwhile, the system is translational invariant. Thus applying the Feynman-Hellman theorem to the GS of the system, we get the expressions for the two kinds of RFSs between two NN spin pairs as

$$\chi_{12} = \frac{4\alpha^2 (\partial_\alpha^2 e_0)^2}{(S - 4e_0 + 4\alpha \partial_\alpha e_0)(S + 1 + 4e_0 - 4\alpha \partial_\alpha e_0)},$$

$$\chi_{23} = \frac{4(\partial_\alpha^2 e_0)^2}{(S - 4\partial_\alpha e_0)(S + 1 + 4\partial_\alpha e_0)}. \quad (29)$$

Obviously, when $S=1/2$, the above expression reduces to Eq. (18). The two RFSs are proportional to the second derivative of the GS energy per spin $e_0 \equiv e_0(\alpha)$. That is, the RFS also has the possibility to signal the second-order QPTs of a mixed-spin system.

Furthermore, it could also be extended to high-spin systems, such as the spin-1 bilinear-biquadratic model, which describes the structure of some materials, such as LiVGe_2O_6 ,^{39,40} and attracts much attention since Haldane⁴¹ predicted that the one-dimensional chain has a spin gap for integer spins. The Hamiltonian reads

$$H_{BB} = \sum_{i=1}^N [\cos \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (30)$$

where \mathbf{S}_i denotes the spin-1 operator, and θ reflects the different coupling strengths. The periodic boundary condition is assumed as well. Obviously, this Hamiltonian is also of SU(2) and translational symmetries. In Eq. (24) of Ref. 38, the QPT of this model is studied by using the RFS between NN-coupling spins, which happens to be proportional to the second derivative of the GS energy density $e_0 \equiv e_0(\theta)$, i.e.,

$$\chi_{12} \propto (e_0 + \partial_\theta^2 e_0)^2. \quad (31)$$

This further confirms that the two-spin RFS is an effective tool in revealing the second-order QPTs even for high-spin systems.

V. CONCLUSION

In conclusion, we have studied the relation between RFS and QPTs. For the spin-1/2 systems with SU(2) symmetry, an expression of RFS based on the spin correlator is derived. Then it is applied to the 1D spin-1/2 dimerized Heisenberg chain. The translational symmetry of this system enables us to establish a direct relation between the RFS and QPTs shown in Eq. (18). Explicitly, the RFS is proportional to the square of the second derivative of the GS energy, which reflects the second-order QPTs of the system. This means the RFS is a good indicator of the second-order QPTs.

In terms of RFS obtained in Eq. (18), we have examined the critical behavior of the 1D spin-1/2 dimerized Heisenberg chain in the antiferromagnetic case. For the GS of the system, two kinds of RFSs between two NN spin pairs are considered both in finite-size and infinite-size situations. It is found that, as the system size increases, the pseudocritical points of the RFSs approach the real critical point $\alpha=1$. In the thermodynamic limit, the critical exponent of the two RFSs is given. These results further convince us that the critical behavior of the system can be reflected by the fidelity susceptibility of its two-spin subsystem, which is of practical use in experiments.

Furthermore, we examine another two systems with high spin, i.e., the mixed-spin dimerized Heisenberg chain and the spin-1 bilinear-biquadratic model, which have the SU(2) and translational symmetries as well. It is also found that the RFS is directly connected to the square of the second derivative of the GS energy. This indicates that, for a broad class of systems with SU(2) and translational symmetries, RFS is effective in identifying second-order QPTs.

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