Fidelity susceptibility approach to quantum phase transitions in the XY spin chain with multisite interactions

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(Received 7 December 2009; published 12 July 2010)

We study the quantum critical behavior of the XY spin chain with multisite interaction by means of a fidelity susceptibility (FS) calculation. The key ingredients (e.g., finite-size scaling behavior, universality principle) of the quantum criticality near the critical point are investigated carefully. The results show that the FS calculation is reliable to characterize the quantum critical behavior and that the multisite interaction can induce the redistribution of the criticality region.

DOI: 10.1103/PhysRevA.82.012308 PACS number(s): 03.67.−a, 64.60.−i, 75.10.Jm

I. INTRODUCTION

At zero temperature, the ground-state (GS) properties of a quantum system may change dramatically owing to the pure quantum fluctuation. This phenomenon, known as quantum phase transition (QPT), is attributed to the interplay between the different orders associated with competing interactions available in the Hamiltonian [1]. This topic attracts much attention in many branches of physics. Traditionally, a QPT is described in the framework of order parameter and symmetry breaking within the Landau-Ginzburg paradigm. In recent years, many works have paid attention to this problem from the quantum-information perspective [2–7]. For example, pairwise entanglement close to the QPT of the one-dimensional Ising model [3] and the entanglement entropy approach to the quantum critical phenomena in XY and XXZ spin chains [5] were addressed. More recently, a concept called fidelity, which is a pure quantum-information notion, has been introduced to investigate the QPT in several spin systems [8–13]. Since there is no need for prior knowledge of the order parameter and symmetry variation in a system under consideration, fidelity seems to be a powerful and universal approach to the QPT [14,15]. Furthermore, in comparison with fidelity, the concept of fidelity susceptibility (FS) can be even more convenient to characterize the QPT, due to its independence of variation of external parameters so long as the variation is not remarkable. In fact, the fidelity susceptibility, as a good tool to investigate the QPT of quite a few of typical systems, such as the Hubbard model [16], the Kitaev honeycomb model [17], the frustrated Heisenberg chain model [18], the extended Harper model [19], and the disordered quantum XY model [20], was employed. In particular, Chen *et al.* [21] investigated the intrinsic relation between the GS fidelity susceptibility and the derivation of the GS energy. They found that the singularity and scaling behavior of the GS fidelity susceptibility are directly related to the derivative of the GS energy, and both of them play an equivalent role in identifying the quantum phase transition. This indicates that the fidelity susceptibility as a nontrivial parameter to characterize the QPT of a quantum system does function.

On other hand, regarding the QPT itself, there has been growing concern with the quantum critical behavior in several exactly solvable quantum spin models with not only the nearest-neighbor spin-spin interactions but also the next-nearest-neighbor ones. Furthermore, the QPT in multiple spin exchange models [22–25], for example, the XX Heisenberg spin chain with $XZY - YZX$ type three-site interaction [23], the spin biaxial model with multiple interaction [24], and the phase diagram of one-dimensional spin XX chain with $XZX + YZY$ type three-site interaction [25], were recently investigated. Comparing those models with only the nearest-neighbor couplings, these models appear to be closer to real situations and exhibit more complicated QPT. For instance, complex and multiple interactions are usually available in transitional metal oxides where the direct exchange between magnetic ions is complimented by superexchange between magnetic ions via nonmagnetic ones. And the additional terms involving the multisite interaction operators were recognized to be important for the theoretical description of many physical systems (e.g., the multiple spin exchange was used for the description of the magnetic properties of solid ^{3}He [26]).

In previous works related to the fidelity susceptibility approach to quantum phase transition, these important and realistic interactions are rarely considered despite such additional interactions often present in a real spin system. In this work, we investigate the fidelity susceptibility associated with the quantum critical properties in an exactly solvable spin chain model with multisite interaction (e.g., $XZX + YZY$ type three-site interaction). The goal of our work is to check whether the fidelity susceptibility can be used to describe the quantum critical behaviors in this specific model, and subsequently how the multisite interaction influences the quantum critical behavior. The two major properties of quantum criticality, that is, the finite-size scaling behavior and universality principle, will be visited both numerically and analytically.

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This article is organized as follows. In Sec. II, we introduce the XY spins model with multisite interaction. By exactly diagonalizing the Hamiltonian, we obtain the expression of the fidelity susceptibility. In Sec. III, the rigorous treatment and numerical computation are carried out to understand the effect of multisite interaction to the quantum critical properties. Finally, we give a summary of our main results.

II. MODEL

We consider the XY model with three-site interaction and the Hamiltonian can be written as

$$H = \sum_l^L J\left(-\frac{1+\gamma}{2}S_l^x S_{l+1}^x - \frac{1-\gamma}{2}S_l^y S_{l+1}^y - \frac{\Omega}{2}S_l^z\right) - \sum_l^L J^*\left(S_{l-1}^x S_l^z S_{l+1}^x + S_{l-1}^y S_l^z S_{l+1}^y\right), \tag{1}$$

where γ is the anisotropy parameter, Ω denotes the external field, and J^* denotes the three-site $XZX + YZY$ type of interaction. By introducing the Jordan-Wigner transformation [1], the Hamiltonian can be rewritten as [25]

$$H = -J\sum_l^L\left[\left(\frac{1}{4}c_l^\dagger c_{l+1} + \frac{\gamma}{4}c_l^\dagger c_{l+1}^\dagger - \frac{\alpha}{4}c_l^\dagger c_{l+2} + \text{H.c.}\right) - \frac{\lambda}{2}\left(c_l^\dagger c_l - \frac{1}{2}\right)\right], \tag{2}$$

where $\lambda = \Omega/J$ and $\alpha = J^*/J$. Without losing generality, we set $\alpha > 0$ hereafter. By introducing the Fourier transforms of the fermionic operators described by $d_k = \frac{1}{\sqrt{L}}\sum_l c_l e^{-i2\pi lk/L}$, we obtain

$$H = \frac{J}{4}\sum_k [2(\cos\kappa - \alpha\cos 2\kappa - \lambda)\, d_k^\dagger d_k - i\gamma\sin\kappa(d_{-k}^\dagger d_k^\dagger + d_{-k}d_k) + \lambda]. \tag{3}$$

Here, $\kappa = 2\pi k/L$. Using the Bogoliubov transformation, the Hamiltonian can be diagonalized as follows,

$$H = \frac{J}{2}\sum_k \varepsilon_k\left(\gamma_k^\dagger\gamma_k - \frac{1}{2}\right), \tag{4}$$

where

$$\varepsilon_k = [(\lambda - \cos\kappa + \alpha\cos 2\kappa)^2 + \gamma^2\sin^2\kappa]^{\frac{1}{2}} \tag{5}$$

and the corresponding Bogoliubov transformed fermion operators are defined as

$$\gamma_k = \cos\frac{\theta_k}{2}d_k - i\sin\frac{\theta_k}{2}d_{-k}^\dagger \tag{6}$$

with angles θ_k satisfying the relation $\tan\theta_k = \gamma\sin\kappa/(\cos\kappa - \lambda - \alpha\cos 2\kappa)$.

The ground state $|g\rangle$ of H, defined as the state annihilated by each operator $\gamma_k(\gamma_k|g\rangle \equiv 0)$, is given as a tensor product of qubitlike state,

$$|g\rangle = \otimes_{k=1}^M\left[\cos\frac{\theta_k}{2}|0\rangle_k|0\rangle_{-k} - i\sin\frac{\theta_k}{2}|1\rangle_k|1\rangle_{-k}\right], \tag{7}$$

where $|0\rangle_k$ and $|1\rangle_k$ are the vacuum and single excitations of the kth mode, respectively. The ground-state fidelity is then defined by $F(q,\delta) = \langle g(q)|g(\widetilde{q})\rangle = \prod_{k=1}^M \cos\frac{\theta_k(q)-\theta_k(\widetilde{q})}{2}$ [9], where q is an arbitrary parameter of the system and $\widetilde{q} = q + \delta$ (δ is a small quantity) denotes the neighboring point to parameter q. Then the FS can be obtained as [21]

$$\chi = \left.\frac{\partial^2 F(q,\delta)}{\partial^2 q}\right|_{\delta=0} = \frac{1}{4}\sum_{k=1}^M\left(\frac{\partial\theta_k}{\partial q}\right)^2, \tag{8}$$

and the FS with respect to λ, γ, and α can be written as follows:

$$\chi_\lambda = \frac{1}{4}\sum_k\frac{[\gamma\sin\kappa]^2}{[(\lambda-\cos\kappa+\alpha\cos 2\kappa)^2+\gamma^2\sin^2\kappa]^2}, \tag{9a}$$

$$\chi_\gamma = \frac{1}{4}\sum_k\frac{[\sin\kappa(\lambda-\cos\kappa+\alpha\cos 2\kappa)]^2}{[(\lambda-\cos\kappa+\alpha\cos 2\kappa)^2+\gamma^2\sin^2\kappa]^2}, \tag{9b}$$

$$\chi_\alpha = \frac{1}{4}\sum_k\frac{[\gamma\sin\kappa\cos 2\kappa]^2}{[(\lambda-\cos k+\alpha\cos 2\kappa)^2+\gamma^2\sin^2\kappa]^2}. \tag{9c}$$

III. FIDELITY SUSCEPTIBILITY AND QPT

We come to look at the quantum criticality as characterized by the fidelity susceptibility and its response to the multisite interaction. In the space of parameters γ and λ, the family of pure XY spin chains exhibit two regions of criticality, defined by the existence of gapless excitations: (i) the XX region of criticality, for $\gamma = 0$ and $\lambda \in (-1,1)$; and (ii) the XY region of criticality given by the lines $\lambda = \pm 1$. Given the two criticality regions, we are allowed to investigate the effect of the multisite interaction on the redistribution of the critical regions.

In Fig. 1(a), we present χ_λ as a function of λ and α with $\gamma = 1.0$ and $L = 10\,001$. The anomaly regions marked by the sharp peaks differ from those identified for the XY spin model without the multisite interaction [9], which corresponds to the case $\alpha = 0$. It is easy to see that the anomaly region shifts from the lines $\lambda = \pm 1$ to the lines $|\lambda + \alpha| = 1$ when this additional interaction emerges ($\alpha > 0$). Figure 1(b) presents the calculated FS χ_λ as a function of λ and γ for a given strength of three-site interaction $\alpha = 0.5$. In comparison with the case of the pure XY model [9], the anomaly regions shift from the lines $|\lambda| = 1$ to the lines $\lambda = -1.5$ and $\lambda = 0.5$, respectively. These results demonstrate the significant influence of the multisite interaction on the location and pattern of the criticality regions in the parameter space.

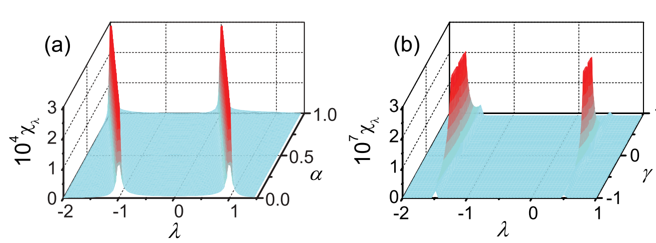

FIG. 1. (Color online) (a) Fidelity susceptibility χ_λ as a function of λ and α. Along the line $|\lambda + \alpha| = 1$, χ_λ exhibits remarkable anomalies; $L = 10\,001$; $\gamma = 1.0$. (b) Fidelity susceptibility χ_λ as a function of λ and γ; $L = 10\,001$; $\alpha = 0.5$. Hereafter, the parameters λ, α, γ, χ_λ, and χ_γ are dimensionless quantities.

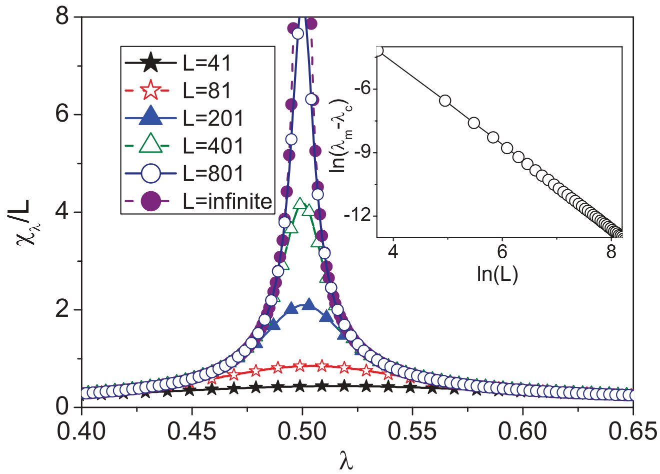

FIG. 2. (Color online) Fidelity susceptibility χ_λ/L as a function of λ. The curves correspond to different lattice sizes $L = 41, 81, 201, 401, 801$, and ∞, respectively. The peak height increases rapidly with increasing L, and the difference between the peak location λ_m and the critical point λ_c can be scaled by $L^{-1.98199}$. Here, $\gamma = 1.0$ and $\alpha = 0.5$.

On the other hand, it is necessary to check whether all these reformational anomaly regions can be regarded as QPT. To proceed, we turn to study the finite-size scaling behavior of χ. The fidelity susceptibility χ_λ/L for different sizes is plotted in Fig. 2. There is no real divergence for finite L, but each curve exhibits marked anomaly (peak) and the peak height increases with lattice size, indicating the finite-size scaling behavior. Along this line, the position λ_m of the peak can be regarded as a pseudocritical point which shifts with L and can be scaled as $L^{-1.98199}$ in approaching the critical point λ_c. It states that $\lambda_m \to \lambda_c$ as $L \to \infty$.

Similar to other approaches for phase transitions, we try to extract the critical exponents from the FS data. For an Ising spin chain, the correlation length around the critical point should satisfy $\xi \sim |\lambda - \lambda_c|^\nu$, where ν is the critical exponent and equals 1 [27]. In most cases, the FS usually depends linearly on the system size, that is, $\chi_\lambda \propto L$ in the noncritical region. Then the averaged FS χ_λ/L, as an intensive quantity in the thermodynamic limit, scales like

$$\frac{\chi_\lambda}{L} \propto \frac{1}{|\lambda_c - \lambda|^\zeta} \tag{10}$$

around the critical point λ_c, with ζ being the corresponding exponent. On the other hand, if the averaged FS around the critical point exhibits a peak for a finite-size system, its maximum point at λ_m scales like

$$\chi_\lambda(\lambda = \lambda_m) \propto L^\mu, \tag{11}$$

and the critical exponent for the correlation length, ν, satisfies the following relation [10]:

$$\zeta = \frac{\mu - 1}{\nu}. \tag{12}$$

In Figs. 3(a) and 3(b), we plot the following expressions alternative to Eqs. (10) and (11):

$$\ln(\chi_\lambda/L) = -\zeta \ln|\lambda_c - \lambda| + c, \tag{13}$$

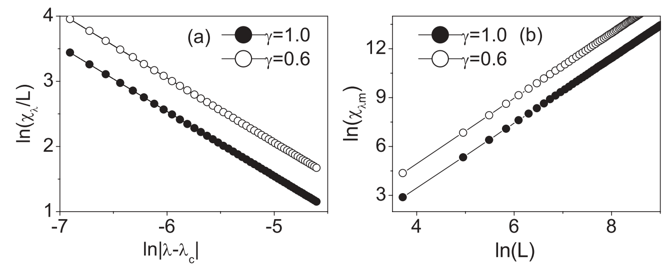

FIG. 3. (a) Plot of $\ln(\chi_\lambda/L)$ against $\ln|\lambda - \lambda_c|$ for evaluating the thermodynamic approaching the critical point. The line slope is -0.98951 (-0.98957) for $\gamma = 1.0$ ($\gamma = 0.6$). (b) The maximum value of $\ln(\chi_\lambda)$, $\ln(\chi_{\lambda_m})$, at the pseudocritical point λ_m as a function of L. The line slope is 1.998 46 (1.998 81) for $\gamma = 1.0$ ($\gamma = 0.6$). The critical exponent ν for the correlation length is determined by the two slopes in (a) and (b) for a fixed γ. Here, $\alpha = 0.5$.

$$\ln(\chi_m) = \mu \ln(L) + c. \tag{14}$$

In Fig. 3(a), the line slopes are -0.98951 and -0.98957 for $\gamma = 1.0$ and $\gamma = 0.6$, respectively. In Fig. 3(b), the line slopes are 1.998 46 and 1.998 81 for $\gamma = 1.0$ and $\gamma = 0.6$, respectively. From Eq. (12), we can obtain the critical exponent ν. In this case, the numerical calculation gives $\nu \sim 1.009$, which is very close to the well-known solution for the Ising model [27]. Given the finite-size scaling ansatz, these results demonstrate convincingly that the quantum critical behavior can be characterized by the FS.

Also, a logarithmic divergence at the critical point must ensue if the the scaling ansatz applies. Taking into account the distance of the maximum of $\ln(\chi_\lambda/L)$ from the critical point, we choose to plot $F = [1 - \exp(\ln(\chi_\lambda/L) - \ln(\chi_\lambda/L)|_{\lambda_m})]$ as a function $L(\lambda - \lambda_m)$ for different lattice sizes. All the data for different L's collapse onto a single curve for the same γ. The numerical results for L ranging from $L = 101$ to $L = 801$ are plotted in Fig. 4, indicating that the critical behavior is scaling invariant, i.e. $\xi/L = \xi'/L'$, and that the critical exponent for the correlation length is $\nu \sim 1$.

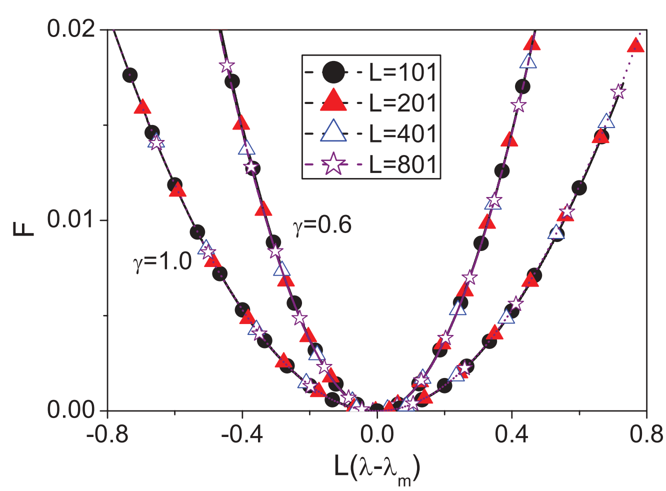

FIG. 4. (Color online) Evaluated $F = [1 - \exp(\ln(\chi_\lambda/L) - \ln(\chi_\lambda/L)|_{\lambda_m})]$ as a function $L(\lambda - \lambda_m)$ for different lattice sizes $L = 101, 201, 401$, and 801. All the data for a fixed parameter γ collapse on a single curve, as expected from the finite-size scaling ansatz. Here, $\alpha = 0.5$ and the parameter F is dimensionless.

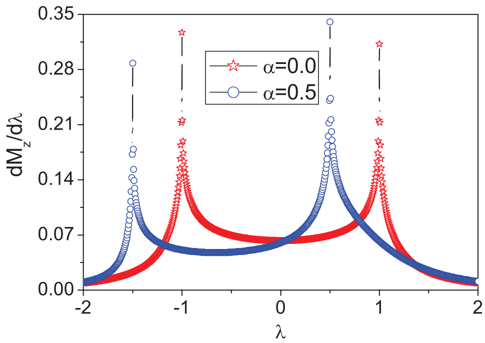

FIG. 5. (Color online) First-order derivative of magnetization $dM_z/d\lambda$, plotted as a function of λ. Here, $L = 10\,001$ and $\gamma = 1.0$. In comparison with the pure Ising spin chain, the peaks of the first-order derivative of magnetization $dM_z/d\lambda$ shift from points $\lambda = \pm 1$ to points $\lambda = -1.5$ and $\lambda = 0.5$, respectively. The unit of quantity $dM_z/d\lambda$ is arb. units.

In addition, we explore the order parameter, magnetization M_z. The mean magnetization M_z is defined as $M_z = \frac{1}{2L}\sum_l \langle g|\sigma_l^z|g\rangle$, where $|g\rangle$ is the ground state of the system. It is easy to obtain M_z:

$$M_z = \frac{1}{2L}\sum_k \frac{\lambda - \cos\kappa + \alpha\cos 2\kappa}{[(\lambda - \cos\kappa + \alpha\cos 2\kappa)^2 + \gamma^2\sin^2\kappa]^{\frac{1}{2}}}. \quad (15)$$

In Fig. 5, we plot the first-order derivation of M_z as a function of λ. For a pure Ising model, there are two marked peaks on the points $\lambda = \pm 1.0$. However, these peaks shift to the points $\lambda = 0.5$ and $\lambda = -1.5$, respectively, when we set $\alpha = 0.5$, demonstrating the effect of multiple interaction on the quantum critical behavior, consistent with previous results.

Furthermore, for a pure $XX(\gamma = 0)$ chain, the critical region appears in $\lambda \in (-1,1)$, where χ_γ exhibits anomaly [9]. In Fig. 6, we plot χ_γ as a function of λ and γ with the three-site interaction $\alpha = 0.5$. It is easy to see that the critical region shifts along the negative direction of the λ axis. At $\alpha = 0.5$, the reform interval for the anomaly shifts to $\lambda \in (-1.5,0.75)$.

The finite-size scaling behavior of χ_γ at $\gamma = 0$ is shown in Fig. 7. We choose two specific points of the peak-structure parts in Fig. 6 with $\lambda = -1.2$ and $\lambda = -1.4$ for a comparison as shown in Figs. 7(a) and 7(b), respectively. The two pictures display a similar structure. Both graphs are constituted

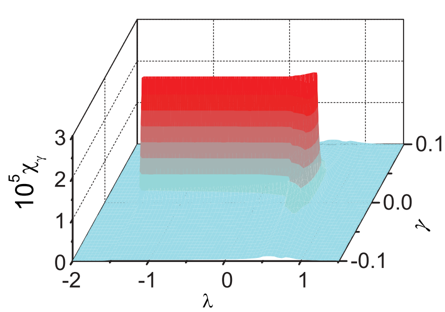

FIG. 6. (Color online) Fidelity susceptibility χ_γ as a function of λ and γ. Here, $L = 10\,001$, $\alpha = 0.5$. In comparison with the pure XX spin chain, the line at which the anomaly appears shifts from the interval $\lambda \in (-1,1)$ to the interval $\lambda \in (-1.5,0.75)$.

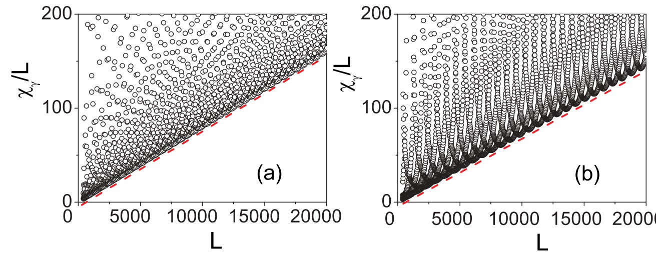

FIG. 7. (Color online) Finite-size scaling behavior of χ_γ at $\gamma = 0.0$: (a) $\lambda = -1.2$ and (b) $\lambda = -1.4$. (The minimum is guided by the dashed red lines.) Here, $\alpha = 0.5$. The system sizes L range from 401 to 20 001 with $\delta L = 4$.

by many curves with oscillation. The minima among the peaks of all the curves grow monotonously with L, and all the data are distributed above the red dashed lines. From these results, we can determine that the value of χ_γ must be infinite when L tends to infinite. Therefore, all the peaks along the anomalous line in Fig. 6 could be regarded as precursors of QPT. On the other hand, we find that these oscillations are caused by the finite-size effect of the system. When $\gamma = 0$, χ_γ can be written as $\chi_\gamma = \sum_k \frac{\sin^2\kappa}{4(\lambda - \cos\kappa + \alpha\cos 2\kappa)^2}$. To make χ_γ a large value or divergent, $\lambda - \cos\kappa + \alpha\cos 2\kappa$ must be very small or tend to zero. If we let $\lambda - \cos\kappa + \alpha\cos 2\kappa = 0$, $\cos(\frac{2\pi k}{L}) = \frac{1\pm\sqrt{1+8\alpha^2-8\alpha\lambda}}{4\alpha}$ must be satisfied. For a finite L, the mode κ is discrete, which induces the peak-style oscillation. When $L \to \infty$, the model κ becomes continuous, and there always exists a model κ_0 such that $\lambda - \cos\kappa_0 + \alpha\cos 2\kappa_0 = 0$; then χ_γ will become divergent. Considering $-1 < \cos\kappa < 1$, for a fixed α, for example, $\alpha = 0.5$, χ_γ presents as divergent in the interval $(-1.5,0.75)$, which is consistent with the numerical results shown in Fig. 6.

IV. SUMMARY

We employ the fidelity susceptibility as a tool to exploit the quantum critical properties in the XY spin chain with multisite interaction (e.g., $XZX + YZY$ type of three-site interaction). Near the critical point, the fidelity susceptibility is singular. A finite-size scaling behavior is investigated for the system with different sizes. This allows us to extract the critical exponent for the correlation length. We also perform numerical calculations to confirm the universality; that is, the critical exponent does not depend on the anisotropic parameter. As a complementarity, we give a brief exploration of the order parameter magnetization M_z. All these major ingredients of the quantum criticality confirm that the FS can be extended to characterize the quantum critical behavior in this system. For a continuous phase transition case, we know that the singularity and scaling behavior of the GS fidelity susceptibility are directly related to the second derivative of the GS energy. In our study, although we take the $\alpha = 0.5$ as a probe, it does not lose generality. All the critical points mark exactly the same order of transition (2nd) as in the XY model. In comparison with the pure XY spin chain, our results show that this additional three-site interaction can induce the redistribution of the critical region for both the $XX(\gamma = 0)$ model and the $XY(\gamma \neq 0)$ ones. On the other hand, from the energy spectrum $\varepsilon_k = [(\lambda - \cos\kappa + \alpha\cos 2\kappa)^2 + \gamma^2\sin^2\kappa]^{\frac{1}{2}}$, we can see that it is non-negative. It can be equal to zero only for the model κ equal to zero or π. So there are two critical values of the magnetic field at which quantum phase transition can take place ($\lambda - 1 + \alpha = 0$ for $\kappa = 0$ and $\lambda + 1 + \alpha = 0$ for $\kappa = \pi$). Consequently, in this special model, this additional interaction cannot produce new critical lines and can only shift the original critical point when it emerges.

ACKNOWLEDGMENTS

The authors acknowledge the financial support from the National Natural Science Foundation of China (Grants No. 50832002 and No. 10874075), the National Key Projects for Basic Researches of China (Grants No. 2006CB921802 and No. 2009CB925101), the Key Projects of Hubei Province (Grant No. D20092204), and the Natural Science Foundation of Hubei Province (Grant No. 2009CDA145).

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