# Scaling properties of fidelity in the spin-1 anisotropic model

Yu-Chin Tzeng and Min-Fong Yang*

*Department of Physics, Tunghai University, Taichung, Taiwan*
(Received 10 September 2007; published 11 January 2008)

By means of the density matrix renormalization group technique, the scaling relation of the fidelity susceptibility proposed recently is verified for the spin-one *XXZ* spin chain with an on-site anisotropic term. Moreover, from the results of both the fidelity susceptibility and the entanglement entropy, the critical points and some of the corresponding critical exponents are determined through a proper finite-size scaling analysis, and these values agree with the findings in the literature. Thus our work provides a numerical support of the use of the fidelity in detecting quantum phase transitions.

Quantum phase transitions (QPTs) [1], driven by purely quantum fluctuations, are characterized by the dramatic changes in the ground state of a many-body system as the controlling parameters in the system Hamiltonian are varied across critical points. Due to latest advances in quantum-information science [2], people attempt to characterize QPTs from the perspective of quantum information. One of the well-studied aspects is to explore the role of quantum entanglement in identifying QPTs [3]. In particular, as a bipartite entanglement measure, the entanglement entropy of a block of length $l$ for one-dimensional systems is shown to exhibit qualitatively different scaling behaviors at and off criticality [4–13]. The entanglement entropy saturates to a finite bound as the length $l$ increases for noncritical (gapped) systems [4–6], whose value can vary for different boundary conditions [7]. However, the entanglement entropy increases logarithmically for critical (gapless) systems [4,8–13]. By using conformal field theory, a universal scaling is expected at a quantum critical point, and its expression depends again on the boundary conditions. Thus the divergent character of the entanglement entropy in the finite-size scaling can faithfully indicate the existence of the critical points for one-dimensional systems.

In the last few years, the ground-state fidelity [14,15] (and its second derivatives, the so-called "fidelity susceptibility" [16]), another concept that emerged from quantum-information science, has attracted much attention because of their application to the analysis of QPTs [15–27]. As illustrated before in several concrete models, it seems that the singularity in the fidelity susceptibility can be an effective tool for detecting critical points. Quite recently general scaling analyses of the fidelity susceptibility were proposed [23,24]. As explicitly shown in Ref. [23], the fidelity susceptibility $\mathcal{S}$ must be bounded above in the thermodynamical limit for noncritical (gapped) systems containing only local operators. However, for critical (gapless) systems of finite size $L$, it fulfills scaling relations

$$\mathcal{S} \sim L^{-\Delta_Q}, \quad \Delta_Q = 2\Delta_V - 2z - d, \tag{1}$$

where $d$ is the spatial dimension, $z$ is the dynamic exponent, and $\Delta_V$ is the scaling dimension of the transition-driving term

in the Hamiltonian. This result implies that the QPTs at those critical points with $\Delta_Q < 0$ can be detected by the power-law divergent behaviors in $\mathcal{S}$.

In this paper, the spin-one *XXZ* spin chain with a uniaxial single-ion anisotropic term is investigated, and we focus our attention on the verification of the predicted scaling behavior of the fidelity susceptibility in Eq. (1). It is known that, while the QPTs can in principle be unveiled by the knowledge of the entanglement entropy and the ground-state fidelity, they are usually difficult to be calculated due to the lack of knowledge of the exact ground-state wave functions. Although numerical exact diagonalization can always be employed to evaluate the entanglement entropy and the fidelity for small systems, this method may not be able to demonstrate the scaling behaviors because of finite-size effects. Thus we need to resort to the density matrix renormalization group (DMRG) technique [28] for the calculations for systems of large sizes. In the present work, both the entanglement entropy and the fidelity susceptibility are evaluated by means of the finite-system DMRG technique under open boundary conditions for system sizes up to $L=160$. In our DMRG calculations, up to 300 states per block are kept and five DMRG sweeps are performed for the truncation error being about $10^{-10}$. We find that developing peaks do appear in both measurements, which signal precursors of the QPTs. Applying a proper finite-size scaling analysis, the proposed scaling relation in Eq. (1) is confirmed numerically. In addition, the critical points in the thermodynamic limit and some of the corresponding critical exponents are determined through a proper finite-size scaling analysis, and these values agree with the results in the literature. Moreover, the results coming from both the entanglement entropy and the fidelity susceptibility are consistent each other. This implies that both measurements are equally suited for revealing QPTs and pinning down the critical points in the present case.

The Hamiltonian for spin-one *XXZ* spin chains of $L$ sites with an on-site anisotropic term is

$$H = \sum_{j=1}^{L-1} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \lambda S_j^z S_{j+1}^z) + D\sum_{j=1}^{L} (S_j^z)^2, \tag{2}$$

where $S_j^\alpha$ ($\alpha=x,y,z$) are the spin-one operators at the $j$th lattice site. $\lambda$ and $D$ parametrize the Ising-like and the uniaxial single-ion anisotropies, respectively. The full phase

*mfyang@thu.edu.tw

diagram consists of six different phases [29,30] (see Refs. [31–33] for recent numerical determinations). On the $\lambda > 0$ half-plane, there consists three phases known as the Haldane, large-$D$, and Néel phases. All these phases show a nonzero energy gap above the ground state. Between these phases, various types of phase transitions take place. There is a Gaussian transition between the Haldane and large-$D$ phases and an Ising transition between the Néel and Haldane phases. These two transitions merge at a tricritical point $\lambda \simeq 3.20$ and $D \simeq 2.90$ [31,32], where the Haldane phase disappears and the Néel–large-$D$ transition becomes first order. Here we consider only the Gaussian and Ising transitions at $\lambda = 1$. In this case, it has been found that, as $D$ is decreased from a large value, one first meets a Gaussian transition from the large-$D$ to Haldane phases at the critical point $D_c \simeq 0.99$, and then an Ising transition from the Haldane to Néel phases at $D_c \simeq -0.31$ [31,33].

For the convenience of the following discussions, some details of the Ising and the Gaussian transitions are reviewed [1]. Both transition lines are of second order with a dynamic exponent $z = 1$. Nevertheless, the former is described by conformal field theory (CFT) with a central charge $c = 1/2$, while the latter by a $c = 1$ CFT [32]. Moreover, their singular behaviors with the universality class of the transition, i.e., critical exponents, can be different. For the Ising transition, the correlation length critical exponent $\nu = 1$ and the scaling dimension of the transition-driving term in the Hamiltonian $\Delta_V = 1$ are known [1]. However, for the Gaussian transition between the Haldane and the large-$D$ phase, it is found that the low-energy effective continuum theory can be described by the sine-Gordon model [32,34]

$$H_{SG} = \frac{1}{2}[\Pi^2 + (\partial_x \Phi)^2] - \frac{\mu}{a^2}\cos(\sqrt{4\pi K}\Phi), \tag{3}$$

where $\Pi$ and $\Phi$ are the conjugate bosonic phase fields, and $a$ is a short-distance cutoff of the order of the lattice spacing. The coefficient $\mu \propto (D - D_c)$ in the vicinity of the critical point $D_c$ for a given $\lambda$, and thus becomes zero at the transition point. The value of the Luttinger-liquid parameter $K$ varies continuously between 1/2 and 2 along the critical line. We note that all the scaling dimensions and the critical exponents are determined by a single parameter $K$. Consequently, they change continuously along the critical line. From sine-Gordon theory [35], it is found that the critical exponent of the correlation length $\nu = 1/(2 - K)$ and the scaling dimension $\Delta_V = K$ for the transition-driving term $\cos(\sqrt{4\pi K}\Phi)$.

In the following, our DMRG results are presented in order [36]. The findings of the fidelity susceptibility $\mathcal{S}(D)$ and the ground-state fidelity $\mathcal{F}(D, D + \delta)$ are shown in Fig. 1. The fidelity susceptibility, or the second derivative of the fidelity, is calculated by [18,20]

$$\mathcal{S}(D) = \lim_{\delta \to 0} \frac{2[1 - \mathcal{F}(D, D + \delta)]}{L\delta^2}, \tag{4}$$

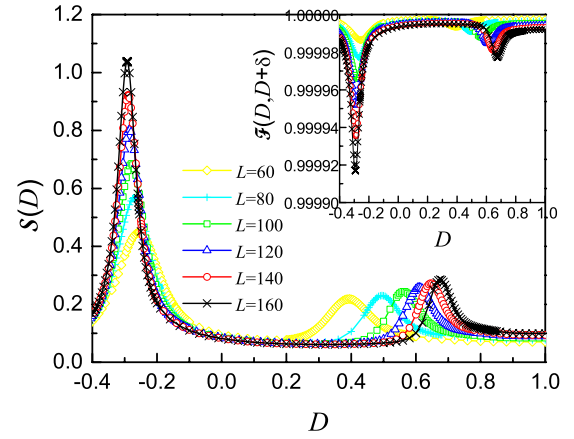where the ground-state fidelity (or the modulus of the overlap) is given by [15,37]



FIG. 1. (Color online) Fidelity susceptibility $\mathcal{S}(D)$ for the spin-1 *XXZ* spin chain in Eq. (2) as functions of $D$ for various sizes $L$ with $\lambda = 1$. The inset shows the fidelity $\mathcal{F}(D, D + \delta)$ as functions of $D$ for the corresponding sizes. Here we take $\delta = 10^{-3}$.

$$\mathcal{F}(D, D + \delta) = |\langle \Psi_0(D) | \Psi_0(D + \delta) \rangle| \tag{5}$$

with $|\Psi_0(D)\rangle$ and $|\Psi_0(D + \delta)\rangle$ being two normalized ground states corresponding to neighboring Hamiltonian parameters. In our calculations, $\delta = 10^{-3}$ is used. As shown in the inset of Fig. 1, drops in the ground-state fidelity are observed, which signal precursors of the Gaussian and the Ising transitions in the model under consideration. The drops in $\mathcal{F}(D, D + \delta)$ at the right-hand side show the Gaussian transition, while those on the left-hand side give the Ising one. Further evidence for indicating QPTs is provided by the results of $\mathcal{S}(D)$. As seen from Fig. 1, the maximum values $\mathcal{S}_{max}$ in the fidelity susceptibility grow with increasing size, and thus indicate divergence in the $L \to \infty$ limit (see also Fig. 4). From the scaling analysis in Ref. [23], these divergent behaviors in $\mathcal{S}$ must imply the appearance of the QPTs. Applying the finite-size scaling, the critical points $D_c$ in the thermodynamic limit can be determined from the locations $D_{max}(L)$ of the local maxima in $\mathcal{S}(D)$ on a size-$L$ system (see Fig. 3).

As mentioned before, the divergent character of the entanglement entropy can also show the existence of the QPTs. Thus the entanglement entropy is evaluated for comparison. Here we consider the entanglement entropy, or the von Neumann entropy of the reduced density matrix $\rho_R(D)$ of the right-hand block of $L/2$ contiguous spins

$$\mathcal{E}(D) = -\mathrm{Tr}[\rho_R(D)\log_2 \rho_R(D)]. \tag{6}$$

Our DMRG results are shown in Fig. 2. It is found that, far away from the critical points, $\mathcal{E}(D)$ has no size dependence, as expected for the gapped phases. Nevertheless, two peaks develop as size $L$ increases. Again, these peaks indicate the existence of the Gaussian and the Ising transitions, and the corresponding critical points $D_c$ can be deduced from the locations $D_{max}(L)$ of the local maxima in $\mathcal{E}(D)$ on a size-$L$ system, as discussed below.
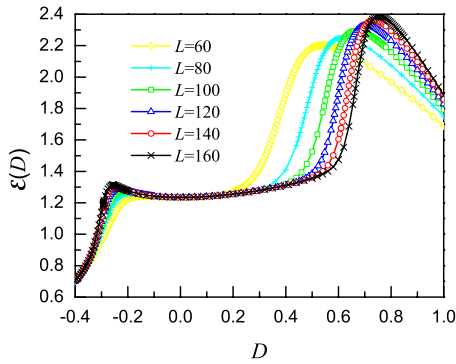
According to the finite-size scaling theory [38], one has

FIG. 2. (Color online) Entanglement entropy $\mathcal{E}(D)$ for the spin-1 *XXZ* spin chain in Eq. (2) as functions of $D$ for various sizes $L$ with $\lambda = 1$.

$$\left| D_{\max}(L) - D_c \right| \propto L^{-1/\nu}, \qquad (7)$$

where $D_c$ is the critical point in the thermodynamic limit and $\nu$ is the critical exponent of the correlation length. Thus $D_c$ can be determined by an extrapolation procedure. The results for the Haldane–large-$D$ and the Haldane-Néel transitions are shown in Fig. 3. For the Gaussian transition between the Haldane and the large-$D$ phases, both extrapolations give
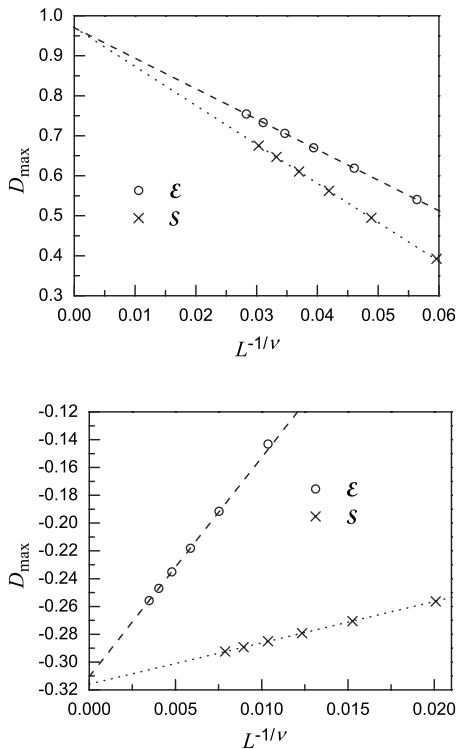




FIG. 3. Finite-size scaling of $D_{\max}$ versus $L^{-1/\nu}$. The full lines are least square straight line fits for sizes with $L \geq 100$. Top: the Haldane–large-$D$ transition, where $\nu \simeq 1.42$ ($\nu \simeq 1.45$) for those $D_{\max}$'s corresponding to the local maxima in the curves of $\mathcal{E}$ ($\mathcal{S}$). Bottom: the Haldane-Néel transition, where $\nu \simeq 0.90$ ($\nu \simeq 1.05$) for those $D_{\max}$'s corresponding to the local maxima in the curves of $\mathcal{E}$ ($\mathcal{S}$).
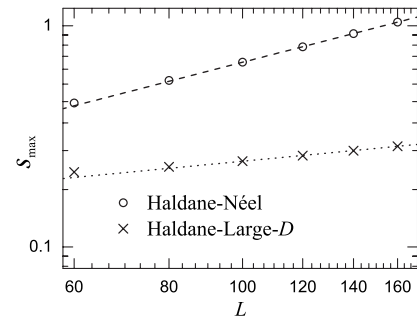


FIG. 4. The log-log plot of $\mathcal{S}_{\max}$ for various sizes $L$. The full lines are least square straight line fits for sizes with $L \geq 100$.

$D_c \simeq 0.97$ as shown in the top panel of Fig. 3. The critical exponent of the correlation $\nu \simeq 1.42$ for the data of $D_{\max}(L)$ obtained from $\mathcal{E}$, while $\nu \simeq 1.45$ for those from $\mathcal{S}$. Because of the relation $\nu = 1/(2-K)$, the Luttinger-liquid parameter $K = 1.30$ ($K = 1.31$) for the data related to $\mathcal{E}$ ($\mathcal{S}$). We find that the values obtained from the measurements of $\mathcal{E}$ and $\mathcal{S}$ agree each other, and they are consistent with the previous findings [32,39], where $D_c \simeq 0.99$ and $K \simeq 1.328$. For the Ising transition between the Néel and the Haldane phases, $D_c \simeq -0.31$ for both extrapolations as shown in the bottom panel of Fig. 3. The critical exponent of the correlation $\nu \simeq 0.90$ for the data of $D_{\max}$ obtained from $\mathcal{E}$, while $\nu \simeq 1.05$ for those from $\mathcal{S}$. Again, the value of $D_c$ agrees with the previous result ($D_c = -0.31$) [33,39], and our findings of $\nu$ are consistent with the theoretical prediction ($\nu = 1$) for the Ising transition. From the above discussions, we find that both the entanglement entropy and the fidelity susceptibility are equally suited for revealing the critical behaviors in the present case.

To verify the predicted critical scaling behavior of the fidelity susceptibility in Eq. (1), the values $\mathcal{S}_{\max}(L)$ of the local maxima for various sizes $L$ are plotted in Fig. 4. It is found that our data do fulfill the scaling relation in Eq. (1), where $\Delta_Q = -0.33$ (i.e., $\Delta_V = 1.34$) for the Gaussian transition and $\Delta_Q = -0.89$ (i.e., $\Delta_V = 1.06$) for the Ising one ($d = 1$ and $z = 1$ are assumed here). The value of $\Delta_V$ for the Ising transition agrees with the predicted one $\Delta_V = 1$. Since $\Delta_V = K$ for the Gaussian transition, the Luttinger liquid parameter $K$ determined by the present finite-size scaling agrees with the previous findings [32] and those determined by the critical exponent $\nu$ coming from the scaling in Fig. 3. Thus the fact that a single parameter $K$ controls all the critical exponents for the Gaussian transition is confirmed by our numerical results.

In summary, the general scaling analysis of the fidelity susceptibility proposed in Ref. [23] is verified by the present DMRG calculations for the model of Eq. (2). The critical points of the Gaussian and the Ising transitions, as well as some of their critical exponents, are determined from the perspective of quantum information. We note that, as seen from Figs. 3 and 4, data for systems of smaller sizes can deviate from the fitting lines obtained from the data for those of larger sizes (say, $L \geq 100$). Therefore, to avoid the finite-size effects and to unveil the correct scaling behaviors at the critical points, calculations for systems of large enough sizes

are necessary. From our DMRG calculation for systems of large sizes, we conclude that the fidelity susceptibility and the entanglement entropy can have similar predictive power for revealing QPTs.

[1] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).

[2] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).

[3] For a recent review, see L. Amico, R. Fazio, A. Osterloh, and J. V. Vedral, arXiv:quant-ph/0703044.

[4] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).

[5] H. Fan, V. Korepin, and V. Roychowdhury, Phys. Rev. Lett. **93**, 227203 (2004).

[6] H. Katsura, T. Hirano, and Y. Hatsugai, Phys. Rev. B **76**, 012401 (2007).

[7] H. Fan, V. Korepin, V. Roychowdhury, C. Hadley, and S. Bose, Phys. Rev. B **76**, 014428 (2007).

[8] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B **424**, 443 (1994).

[9] V. E. Korepin, Phys. Rev. Lett. **92**, 096402 (2004).

[10] P. Calabrese and J. Cardy, J. Stat. Mech.: Theory Exp. 2004, P06002.

[11] N. Laflorencie, E. S. Sørensen, M. S. Chang, and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006).

[12] H. Q. Zhou, T. Barthel, J. O. Fjærestad, and U. Schollwöck, Phys. Rev. A **74**, 050305(R) (2006).

[13] For a recent review, see J. Cardy, e-print arXiv:0708.2978.

[14] H. T. Quan, Z. Song, X. F. Liu, P. Zanardi, and C. P. Sun, Phys. Rev. Lett. **96**, 140604 (2006).

[15] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006).

[16] W. L. You, Y. W. Li, and S. J. Gu, Phys. Rev. E **76**, 022101 (2007).

[17] P. Zanardi, M. Cozzini, and P. Giorda, J. Stat. Mech.: Theory Exp. 2007, L02002.

[18] M. Cozzini, P. Giorda, and P. Zanardi, Phys. Rev. B **75**, 014439 (2007).

[19] M. Cozzini, R. Ionicioiu, and P. Zanardi, Phys. Rev. B **76**, 104420 (2007).

[20] P. Buonsante and A. Vezzani, Phys. Rev. Lett. **98**, 110601 (2007).

[21] N. Oelkers and J. Links, Phys. Rev. B **75**, 115119 (2007).

[22] P. Zanardi, P. Giorda, and M. Cozzini, Phys. Rev. Lett. **99**, 100603 (2007).

[23] L. Campos Venuti and P. Zanardi, Phys. Rev. Lett. **99**, 095701 (2007).

[24] S. J. Gu, H. M. Kwok, W. Q. Ning, and H. Q. Lin, e-print arXiv:0706.2495.

[25] S. Chen, L. Wang, S. J. Gu, and Y. Wang, Phys. Rev. E **76**, 061108 (2007).

[26] H. Q. Zhou and J. P. Barjaktarevic, e-print arXiv:cond-mat/0701608; H. Q. Zhou, J. H. Zhao, and B. Li, e-print arXiv:0704.2940; H. Q. Zhou, e-print arXiv:0704.2945.

[27] M. F. Yang, Phys. Rev. B **76**, 180403(R) (2007).

[28] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993); U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

[29] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).

[30] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).

[31] W. Chen, K. Hida, and B. C. Sanctuary, Phys. Rev. B **67**, 104401 (2003).

[32] C. Degli Esposti Boschi, E. Ercolessi, F. Ortolani, and M. Roncaglia, Eur. Phys. J. B **35**, 465 (2003).

[33] L. Campos Venuti, C. Degli Esposti Boschi, E. Ercolessi, G. Morandi, F. Ortolani, S. Pasini, and M. Roncaglia, Eur. Phys. J. B **53**, 11 (2006).

[34] Here we use the notations of Ref. [32].

[35] S. Lukyanov and A. Zamolodchikov, Nucl. Phys. B **493**, 571 (1997).

[36] To lift the double degeneracy in the Néel phase, a Zeeman term $h_1 S_1^z$ acting only upon the spin at site 1 is added in the Hamiltonian of Eq. (2). Here we take the boundary magnetic field $h_1 = -0.01$. The inclusion of this tiny Zeeman splitting selects a specific ground state and stabilizes our calculations of the fidelity in the Néel phase. Nevertheless, this term is found to have no significant effect on the entanglement entropy and the fidelity in other phases.

[37] The DMRG method had been used to calculate the overlap of two different ground states for a decade. For example, people had applied this technique to evaluate the exponent of the orthogonality catastrophe for the problem of a single impurity in a one-dimensional Luttinger liquid. S. Qin, M. Fabrizio, and L. Yu, Phys. Rev. B **54**, R9643 (1996); S. Qin, M. Fabrizio, L. Yu, M. Oshikawa, and I. Affleck, *ibid.* **56**, 9766 (1997). For a recent review, see I. P. McCulloch, J. Stat. Mech.: Theory Exp. 2007, P10014.

[38] M. E. Fisher and M. N. Barber, Phys. Rev. Lett. **28**, 1516 (1972); M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, London, 1983), Vol. 8, p. 145.

[39] We note that the DMRG calculations in Refs. [32] and [33] are under the periodic boundary conditions, rather than the open boundary conditions used in the present work. The small discrepancy of our results from theirs may be due to the different boundary conditions employed.