Fidelity susceptibility in the two-dimensional transverse-field Ising and *XXZ* models

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We study the fidelity susceptibility in the two-dimensional (2D) transverse-field Ising model and the 2D *XXZ* model numerically. It is found that in both models, the fidelity susceptibility as a function of the driving parameter diverges at the critical points. The validity of the fidelity susceptibility to signal for the quantum phase transition is thus verified in these two models. We also compare the scaling behavior of the extremum of the fidelity susceptibility to that of the second derivative of the ground-state energy. From those results, the theoretical argument that fidelity susceptibility is a more sensitive seeker for a second-order quantum phase transition is also testified in the two models.

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I. INTRODUCTION

Fidelity, a concept emerging from quantum information theory, has recently become an attractive approach toward the study of critical phenomena in condensed-matter physics. In a quantum many-body system, the quantum phase transition is completely driven by the quantum fluctuation in the ground state and is incarnated by an abrupt change in the qualitative structure of the ground-state wave function as the system varies across the critical point [1]. Therefore, being a measure of the similarity between two states, the fidelity is expected to show a dramatic change across the transition points. This motivated people to start exploring its role played in quantum phase transitions [2–4]. Moreover, as the fidelity can be viewed as a space geometrical quantity, no *a priori* knowledge of the order parameter and symmetry breaking of the system is required. This is thus a great advantage to the study of quantum phase transitions using fidelity approaches.

Following the streamline of fidelity, some alternative schemes, such as the fidelity susceptibility [5], fidelity per site [6], operator fidelity [7], and density-functional fidelity [8], have been proposed. As to establish a closer picture to condensed-matter physics, we follow the concept of fidelity susceptibility in this paper. Mathematically, the fidelity susceptibility is just the leading term of the fidelity. It defines the response of the fidelity to the driving parameter. As a result, the singularity of the fidelity across the transition points could thus be reflected in the divergence of the fidelity susceptibility. In fact, this argument has been consolidated by the results in a number of one-dimensional quantum many-body systems [9] (see also a review article [10]).

In this paper, we investigate the behavior of the fidelity susceptibility in two two-dimensional (2D) models, namely, the 2D transverse-field Ising model and the *XXZ* model, numerically. Our results show that the fidelity susceptibility as a function of the driving parameter diverges at the quantum phase-transition points in both models. The scaling behaviors of the extremum of the fidelity susceptibility at the transition point and that of the second derivative of the ground-state energy are also compared. From those results, the theoretical argument that the fidelity susceptibility is a more sensitive indicator than the second derivative of the ground-state energy in searching for a second-order quantum phase transition is testified. Besides, it is also found that the fidelity susceptibility shows a scaling behavior in the vicinity of the critical point and its critical exponents for both models are also obtained through finite-size scaling analysis.

II. FORMULISM

For a general form of the Hamiltonian,

$$H(\lambda) = H_0 + \lambda H_I, \tag{1}$$

where H_I is the driving Hamiltonian and λ denotes its strength. The fidelity is the modulus of the overlap between two ground states $|\Psi_0(\lambda)\rangle$ and $|\Psi_0(\lambda+\delta\lambda)\rangle$ [3],

$$F(\lambda,\lambda+\delta\lambda) = |\langle\Psi_0(\lambda)|\Psi_0(\lambda+\delta\lambda)\rangle|. \tag{2}$$

Since our focus is on continuous quantum phase transitions, the ground state of the Hamiltonian is nondegenerated for a finite system. $|\Psi_0(\lambda+\delta\lambda)\rangle$ can thus be obtained from the time-independent nondegenerated perturbation theory. Extracting the leading term of the fidelity, the fidelity susceptibility can be expressed as [5,11]

$$\chi_F(\lambda) = \sum_{n\neq 0} \frac{|\langle\Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle|^2}{[E_n(\lambda)-E_0(\lambda)]^2}, \tag{3}$$

where $|\Psi_n(\lambda)\rangle$ is a set of orthogonal basis satisfying $H(\lambda)|\Psi_n(\lambda)\rangle = E_n(\lambda)|\Psi_n(\lambda)\rangle$. On the other hand, consider the second derivative of the ground-state energy with respect to λ [12],

$$\frac{\partial^2 E_0(\lambda)}{\partial\lambda^2} = \sum_{n\neq 0} \frac{2|\langle\Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle|^2}{E_0(\lambda)-E_n(\lambda)}, \tag{4}$$

one may easily realize that the above expression is very similar to the perturbation form of fidelity susceptibility in Eq. (3) except having different exponent in the denominator. Therefore, one may expect that both the singularity of fidel-

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ity susceptibility and the second derivative of the ground-state energy are intrinsically due to the vanishing of the energy gap in the thermodynamic limit [12]. However, the difference in the exponent of the dominator makes fidelity susceptibility a more sensitive quantity in searching for quantum phase transitions. That is to say, while the fidelity susceptibility shows a divergence at the critical point, the second derivative of the ground-state energy may still be a continuous function.

Furthermore, to study the scaling behavior of the fidelity susceptibility around the critical point, we may perform finite-size scaling analysis [13,14]. Let us consider a system consisting of N sites such that $N=L^d$, where d is the real dimension of the system. Around the critical point λ_c, the fidelity susceptibility behaves as

$$\frac{\chi_F(\lambda)}{L^{d_a^{\pm}}} \sim \frac{1}{|\lambda_c - \lambda|^{\alpha^{\pm}}}, \tag{5}$$

where $\alpha^+(\alpha^-)$ is the critical exponent of the fidelity susceptibility above (below) the critical point, $d_a^{\pm}$ is the quantum adiabatic dimension, and hence $\chi_F(\lambda)/L^{d_a^{\pm}}$ is an intensive quantity. For a finite system, if the fidelity susceptibility shows a peak at a certain point $\lambda_{\max}$, its maximum value scales like

$$\chi_F(\lambda_{\max}) \sim L^{d_a^c}, \tag{6}$$

where d_a^c is the critical adiabatic dimension. The above two asymptotic behaviors satisfy [14]

$$\frac{\chi_F(\lambda,L)}{L^{d_a^{\pm}}} = \frac{A}{L^{-d_a^c+d_a^{\pm}} + B(\lambda - \lambda_{\max})^{\alpha^{\pm}}}, \tag{7}$$

where A is a constant, B is a nonzero function of λ, and both of them are independent of the system size. From Eq. (7), one can find that the rescaled fidelity susceptibility is a universal function of $L^{\nu}(\lambda-\lambda_{\max})$,

$$\frac{\chi_F(\lambda_{\max},L) - \chi_F(\lambda,L)}{\chi_F(\lambda,L)} = f[L^{\nu}(\lambda - \lambda_{\max})], \tag{8}$$

where ν is the critical exponent of the correlation length. The critical exponent of the fidelity susceptibility can then be obtained as [14,15]

$$\alpha^{\pm} = \frac{d_a^c - d_a^{\pm}}{\nu}. \tag{9}$$

III. TWO-DIMENSIONAL TRANSVERSE-FIELD ISING MODEL

The Hamiltonian of the 2D transverse-field Ising model [16,17] defined on a square lattice reads

$$H_{\text{Ising}} = -\sum_{\langle \mathbf{ij} \rangle} S_{\mathbf{i}}^x S_{\mathbf{j}}^x - \frac{h}{2}\sum_{\mathbf{i}} S_{\mathbf{i}}^z, \tag{10}$$

where $S_{\mathbf{i}}^x$, $S_{\mathbf{i}}^y$, and $S_{\mathbf{i}}^z (S_{\mathbf{i}}^{\kappa}=\sigma_{\mathbf{i}}^{\kappa}/2, \kappa=x,y,z)$ are spin-1/2 operators at site $\mathbf{i}$, h is the transverse-field strength in unit of the Ising coupling, and the sum $\langle\ \rangle$ runs over the nearest-neighboring pairs on the lattice. Periodic boundary conditions are assumed. This model was originally introduced by de Gennes to describe potassium-dihydrogen-phosphate-type ferroelectrics [16] and has been studied extensively via various approaches, such as real-space renormalization group [18], density-matrix renormalization [19], numerical diagonalization [20,21], and entanglement [22].

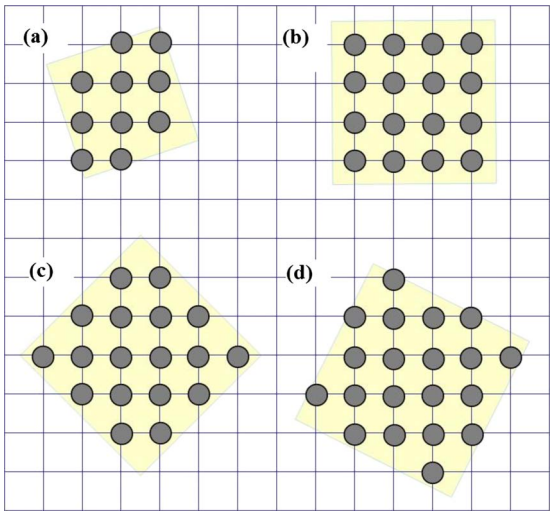

FIG. 1. (Color online) Two-dimensional structures for different system sizes $N=10,16,18,20$ which can be placed on a square lattice with periodic boundary conditions.

Obviously, the Hamiltonian of the model commutes with the parity operator $P=\Pi_{\mathbf{i}}\sigma_{\mathbf{i}}^z$. Thus, each eigenstate of the Hamiltonian is also an eigenstate of P. The Hilbert space can then be decomposed into subspace $V(p)$, where p is the eigenvalue of P and is specified in each subspace. For a finite system, the ground state of the Ising model is nondegenerated in each subspace, thus the perturbation expansion as introduced in the previous section is valid as long as the lattice is finite. In the thermodynamic limit, the model exhibits a quantum phase transition at $1/h_c \simeq 0.328$ [20,21]. For $h \gg h_c$, the transverse field dominates and the ground state is a paramagnetic phase, with spins almost fully polarized in the z direction. For $h \ll h_c$, the ground state is a ferromagnetic phase and is doubly degenerated.

To study a model on a two-dimensional square lattice with periodic boundary conditions, we need to construct proper lattice structures that are suitable for exact diagonalization. In this paper, we will diagonalize two models with system sizes $N=10,16,18,20$, whose structures are shown in Fig. 1. The effective length $L=\sqrt{N}$ might then be a real number instead of an integer.

Figure 2 shows the numerical result of the fidelity susceptibility of the Ising model on a square lattice for various system sizes. It can be seen that on both sides around the critical point, the averaged fidelity susceptibility is an intensive quantity, i.e., $\chi_F \sim N \sim L^2$, and we have $d_a^{\pm}=2$. More importantly, the averaged fidelity susceptibilities for different N all show a peak at $h_{\max}$. This peak position of the fidelity susceptibility $h_{\max}$ is plotted as a function of $1/N$, as shown in the inset of Fig. 2. The linear fitting gives

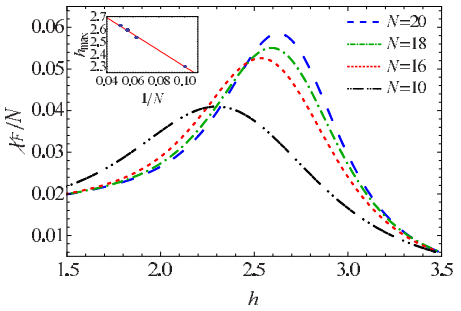

FIG. 2. (Color online) The averaged fidelity susceptibility in the ground state of the 2D transverse-field Ising model on a square lattice as a function of h. Inset shows $h_{\max}$ as a function of $1/N$. The y intercept of the line is 2.95 ± 0.01.

$$h_{\max} = 2.95 - \frac{6.56}{N}.$$

In the thermodynamic limit, we obtain

$$h_c = 2.95 \pm 0.01,$$

which gives $1/h_c = 0.326 \pm 0.001$. Comparing this value to the critical point $1/h_c \simeq 0.328$ obtained in previous works [20,21], our result here is consistent with them up to two digits.

Moreover, we can also see that the averaged fidelity susceptibility peaks sharper for a larger N and is in fact scales approximately with $N^{0.51}$ as shown in the inset of Fig. 4. Physically, as the ground-state wave function of the model changes abruptly across the transition point, the fidelity susceptibility, as a measure of the leading response of the fidelity to the driving parameter, is intuitively expected to show a divergence at the critical point. Here, we have shown numerically that this is in fact the case and verified the significance of fidelity susceptibility in signaling for the quantum phase transition in the 2D Ising model.

Figure 3 shows the second derivative of the averaged ground-state energy of the Ising model for several system sizes of a square lattice as a function of h. As it is well known that the Ising model exhibits a second-order phase transition, the second derivative of the averaged ground-state

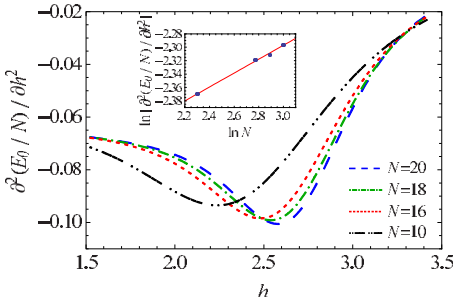

FIG. 3. (Color online) The second derivative of the averaged ground-state energy of the 2D transverse-field Ising model on a square lattice as a function of h. Inset shows the scaling behavior of the minimum of the second derivative of the averaged ground-state energy. The slope of the line is approximately 0.103.

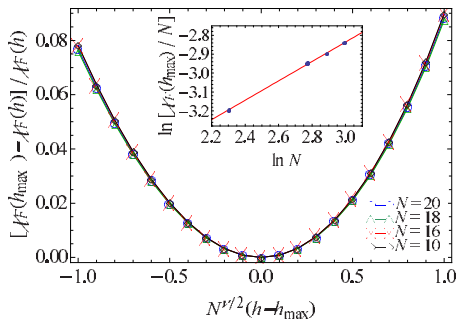

FIG. 4. (Color online) The finite-size scaling analysis is performed for the case of power-law divergence for the 2D transverse-field Ising model. The fidelity susceptibility for different system sizes is a function of $N^{\nu/2}(h-h_{\max})$ only, with the critical exponent $\nu \simeq 1.40$. Insert shows the scaling behavior of the maximum of the averaged fidelity susceptibility. The slope of the line is 0.51.

energy is expected to show a minimum at the transition point. From the inset of Fig. 3, it is found that the minimum value of the second derivative of the averaged ground-state energy scales approximately with $N^{0.103}$. Comparing this value to that of the fidelity susceptibility, which is about $0.51 (d_a^c \simeq 3.02)$, we may conclude that the fidelity susceptibility is a more sensitive tool in detecting for a second-order quantum phase transition.

Figure 4 shows the finite-size scaling analysis in the case of power-law divergence of the 2D transverse-field Ising model. The rescaled fidelity susceptibility collapsed to a single curve for various system sizes. The critical exponent of the correlation length can thus be obtained as $\nu \simeq 1.40$. Together with the slope of the line in the inset of Fig. 4 and from Eq. (9), the critical exponent of the fidelity susceptibility is found to be

$$\alpha = \frac{1.02}{1.40} \simeq 0.73.$$

IV. TWO-DIMENSIONAL *XXZ* MODEL

For the 2D XXZ model, the Hamiltonian is given by

$$H_{XXZ} = \sum_{\langle \mathbf{ij} \rangle} (S_{\mathbf{i}}^x S_{\mathbf{j}}^x + S_{\mathbf{i}}^y S_{\mathbf{j}}^y + \Delta S_{\mathbf{i}}^z S_{\mathbf{j}}^z), \tag{11}$$

where $\Delta = J_z/J_y (J_x = J_y)$ is the dimensionless parameter characterizing the anisotropy of the model. The sum is over all the nearest neighbors on a square lattice. Again, periodic boundary conditions are assumed. For the XXZ model in two dimensions, there exists no exact solution. One has to use either approximate analytical approach such as the spin-wave theory or numerical approach such as exact diagonalization studies of a finite lattice. For the latter approach, to obtain results in the thermodynamic limit, finite-size scaling analysis must be performed [23,24]. Therefore, a physical quantity which is more sensitive to the system size than the traditional second derivative of the ground-state energy would be very useful to study the critical phenomena numerically.

From Eq. (11), it can be easily seen that the Hamiltonian of the XXZ model commutes with the z component of total

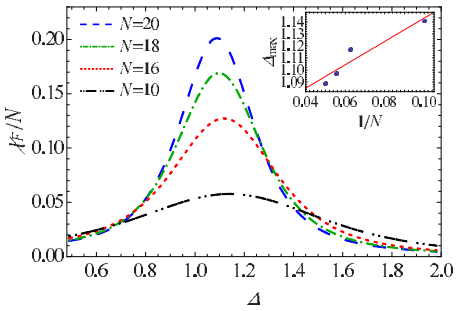

FIG. 5. (Color online) The averaged fidelity susceptibility in the ground state of the 2D *XXZ* model on a square lattice as a function of Δ. Inset shows Δ_{max} as a function of $1/N$. The y intercept of the line is 1.05 ± 0.02.

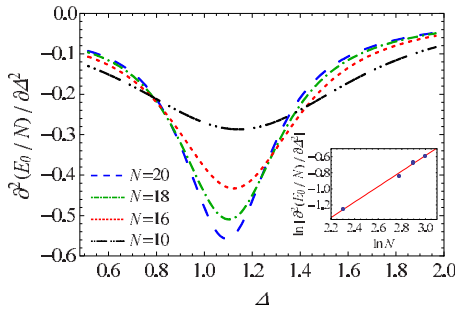

FIG. 6. (Color online) The second derivative of the averaged ground-state energy of the 2D *XXZ* model as a function of Δ. Inset shows the scaling behavior of the minimum of the second derivative of the averaged ground-state energy. The slope of the line is approximately 0.96.

spin operator $S^z_{\text{total}}=\Sigma_{\mathbf{i}}S^z_{\mathbf{i}}$. Thus, each eigenstate of the Hamiltonian is also an eigenstate of S^z_{total}. The Hilbert space can then be decomposed into numerous subspaces $V(M)$, where M is the eigenvalue of S^z_{total}. For a finite sample, the ground state of the *XXZ* model is nondegenerated in any of the admissible subspace $V(M)$ [25,26]. Therefore, the perturbation expansion can also be applied to this model as long as the system is finite. In the thermodynamic limit, the quantum phase transition takes place at the isotropic point $\Delta_c=1$. This phenomenon can be understood by the picture of the first-excited energy levels crossing at the transition point [27]. For $\Delta \gg \Delta_c$, the last term in the Hamiltonian dominates and the ground state is an antiferromagnetic phase along the z direction. For $\Delta \ll \Delta_c$, the first two terms in the Hamiltonian dominate and the ground state is also an antiferromagnetic phase, but in the xy plane. It is well known that long-range orders are present in both of the two phases. However, whether there's a long-range order at the critical point is still an open question. With the help of fidelity susceptibility, we may also find some hints toward this question.

The numerical result of the averaged fidelity susceptibility for various system sizes of the 2D *XXZ* model on a square lattice as a function of Δ is shown in Fig. 5. The averaged fidelity susceptibility is an intensive quantity, meaning that $\chi_F \sim N$, on both sides of the critical point. Moreover, like the previous case of the Ising model, the averaged fidelity susceptibility of the *XXZ* model also shows a peak at $\Delta_{\max}$. The inset of Fig. 5 shows the peak position of the fidelity susceptibility $\Delta_{\max}$ as a function of $1/N$. The linear fitting gives

$$\Delta_{\max} = 1.05 + \frac{0.97}{N}.$$

In the thermodynamic limit, we obtain

$$\Delta_c = 1.05 \pm 0.02.$$

Comparing to the theoretical critical point $\Delta_c=1$, our result here is consistent up to two digits.

Besides, from the slope of the straight line in the inset of Fig. 7, it is found that the peak of the averaged fidelity susceptibility scales with the system size like $N^{1.81}$. Therefore, one may expect the fidelity susceptibility to show a singularity at the critical point in the thermodynamic limit. Hence, the validity of the fidelity susceptibility as a seeker for the quantum phase transition is also verified in the 2D *XXZ* model. Nevertheless, following the idea of the implication of existence of long-range correlation from the divergence of the fidelity susceptibility [28], we argue that long-range correlation is in fact present at the transition point of the 2D *XXZ* model. This is also in agreement with the previous conclusion drawn from the study of the 2D *XXZ* model using entanglement [29].

In comparison, the second derivative of the averaged ground-state energy for various system sizes exhibits a minimum at the transition point, as shown in Fig. 6. From the inset of Fig. 6, it is also found that the minimum value of the second derivative of the averaged ground-state energy scales approximately with $N^{0.96}$, meaning that it shows a slower divergence at the critical point compared to the fidelity susceptibility. In other words, the fidelity susceptibility is again a more sensitive candidate in seeking for the quantum phase transition in the 2D *XXZ* model.

Figure 7 shows the finite-size scaling analysis in the case of power-law divergence of the 2D *XXZ* model. The rescaled fidelity susceptibility almost collapsed to a single curve for a large-enough system size, say $N>10$. The exponent of the correlation length is obtained as $\nu \simeq 3.00$. From the slope of the inset in Fig. 7 and using Eq. (9), the critical exponent of the fidelity susceptibility is calculated to be

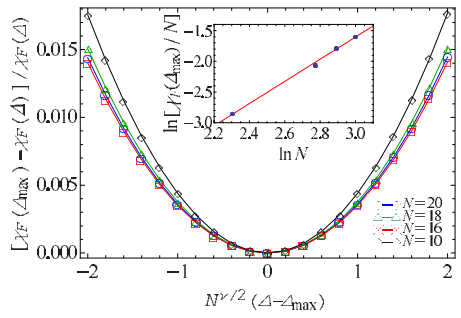

FIG. 7. (Color online) The finite-size scaling analysis is performed for the case of power-law divergence for the 2D *XXZ* model. The fidelity susceptibility for $N>10$ is a function of $N^{\nu/2}(\Delta-\Delta_{\max})$ only, with the critical exponent $\nu \simeq 3.00$. Inset shows the scaling behavior of the maximum of the averaged fidelity susceptibility. The slope of the line is 1.81.

$$\alpha = \frac{3.62}{3.00} = 1.21.$$

V. SUMMARY

To conclude, through the numerical study of the fidelity susceptibility in the 2D transverse-field Ising model and the 2D *XXZ* model, we found that the fidelity susceptibility as a function of the driving parameter diverges in both models at the critical point. By comparing the scaling behavior of the extremum of the fidelity susceptibility to that of the second derivative of the ground-state energy, we also showed that fidelity susceptibility is a more sensitive indicator in detecting for a second-order quantum phase transition. By performing finite-size scaling analysis, the critical exponents of the fidelity susceptibility in both models are also obtained. Finally, due to the divergence of fidelity susceptibility in the 2D *XXZ* model, we argued that the system shows a long-range correlation at the critical point of the model.

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