Fidelity, dynamic structure factor, and susceptibility in critical phenomena

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Motivated by the growing importance of fidelity in quantum critical phenomena, we establish a general relation between the fidelity and structure factor of the driving term in a Hamiltonian through the concept of fidelity susceptibility. Our discovery, as shown by some examples, facilitates the evaluation of fidelity in terms of susceptibility using well-developed techniques, such as density matrix renormalization group for the ground state, or Monte Carlo simulations for the states in thermal equilibrium.

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I. INTRODUCTION

Recently, much attention [1–6] has been drawn to the role of fidelity, a concept emerging from quantum-information theory [7], in quantum critical phenomena [8]. Since fidelity is a measure of similarity between states, a dramatic change in the structure of the ground state around the quantum critical point should result in a great difference between the two ground states on the both sides of the critical point. For example, in the one-dimensional *XY* model, the fidelity shows a narrow trough at the phase transition point [2]. Similar properties were also found in fermionic [3] and bosonic systems [5]. As fidelity is purely a quantum-information concept, these works actually established a connection between quantum-information theory and condensed matter physics.

However, except for a few specific models, such as the one-dimensional *XY* model and the Dicke model [1,2], it is tedious to evaluate fidelity from the ground-state wave functions. Therefore, a neater and simpler formalism is of great importance for the extensive application of fidelity to critical phenomena. For this purpose, we introduce the concept of fidelity susceptibility, which defines the response of fidelity to the driving parameter of the Hamiltonian. At zero temperature, we show that the fidelity susceptibility is intrinsically related to the dynamic structure factor of the driving Hamiltonian, namely, H_I, that causes the quantum phase transition. Based on some well-developed numerical techniques for the ground-state properties, such as exact diagonalization (ED) [9] and density matrix renormalization group (DMRG) [10], a scheme is proposed to evaluate the dynamic structure factor of H_I. On the other hand, starting from the definition of the fidelity of a thermal state, we show that the fidelity susceptibility is simply the thermal fluctuation term, such as the specific heat C_v for the internal energy and the magnetic susceptibility χ for magnetization. These can easily be obtained from Monte Carlo simulations [11].

II. GROUND-STATE FIDELITY AND DYNAMIC STRUCTURE FACTOR

The general Hamiltonian of quantum many-body systems reads

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

where H_I is the driving Hamiltonian and λ denotes its strength. The eigenstates $|\Psi_n(\lambda)\rangle$ that satisfy $H(\lambda)|\Psi_n(\lambda)\rangle = E_n|\Psi_n(\lambda)\rangle$ define a set of orthogonal complete bases in the Hilbert space. Here we restrict ourselves to the phase transition, which is not induced by the ground-state level crossing. That means the ground state of the Hamiltonian is nondegenerate for a finite system. Next we change $\lambda \to \lambda + \delta\lambda$, where $\delta\lambda$ is so small that perturbation is applicable. To the first order, the ground state becomes

$$|\Psi_0(\lambda + \delta\lambda)\rangle = |\Psi_0(\lambda)\rangle + \delta\lambda \sum_{n\neq 0} \frac{H_{n0}(\lambda)|\Psi_n(\lambda)\rangle}{E_0(\lambda) - E_n(\lambda)} \tag{2}$$

and

$$H_{n0} = \langle \Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle. \tag{3}$$

Following Ref. [2], the fidelity is defined as the overlap between $|\Psi_0(\lambda)\rangle$ and $|\Psi_0(\lambda+\delta\lambda)\rangle$, that is,

$$F_i(\lambda, \delta) = |\langle \Psi_0(\lambda)|\Psi_0(\lambda + \delta)\rangle|. \tag{4}$$

Therefore, to the lowest order, we have

$$F_i^2 = 1 - \delta\lambda^2 \sum_{n\neq 0} \frac{|\langle \Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle|^2}{[E_n(\lambda) - E_0(\lambda)]^2} + \cdots. \tag{5}$$

Clearly, the fidelity is $\delta\lambda$ dependent and so it is an artificial quantity. Despite this, we can still see from Eq. (5) that the most relevant term in determining fidelity is its second derivative. Compared with linear response theory, the coefficient term before $\delta\lambda^2$ actually defines the response of fidelity to a small change in λ. From this point of view, we introduce the concept of *fidelity susceptibility* as

$$\chi_F \equiv \lim_{\delta\lambda\to 0} \frac{-2 \ln F_i}{\delta\lambda^2}. \tag{6}$$

With Eq. (5), it can be rewritten as

$$\chi_F(\lambda) = \sum_{n\neq 0} \frac{|\langle \Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle|^2}{[E_n(\lambda) - E_0(\lambda)]^2} \tag{7}$$

in the ground state. We would like to point out that, although the aforementioned procedure is based on perturbation theory, the fidelity susceptibility (7) depends only on the

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spectra of the Hamiltonian $H(\lambda)$ and the hopping matrix H_{n0}. Unfortunately, except for some very small systems which are usually far away from the scaling region, Eq. (7) is almost not computable, due to the lack of knowledge of the set of eigenstates. In order to overcome the difficulty, it is necessary to consider the time evolution of the system. For simplicity, we omit the parameter λ in the following expressions. Define the *dynamic fidelity susceptibility* as

$$\chi_F(\omega) = \sum_{n\neq 0} \frac{|\langle \Psi_n|H_I|\Psi_0\rangle|^2}{(E_n - E_0)^2 + \omega^2}. \tag{8}$$

Performing a Fourier transformation and taking derivative, we then obtain

$$\frac{\partial \chi_F(\tau)}{\partial \tau} = -\pi[\langle \Psi_0|H_I(\tau)H_I(0)|\Psi_0\rangle - \langle \Psi_0|H_I|\Psi_0\rangle^2]\theta(\tau) + \pi[\langle \Psi_0|H_I(0)H_I(\tau)|\Psi_0\rangle - \langle \Psi_0|H_I|\Psi_0\rangle^2]\theta(-\tau), \tag{9}$$

with τ being the imaginary time and

$$H_I(\tau) = e^{H(\lambda)\tau} H_I e^{-H(\lambda)\tau}. \tag{10}$$

The two equations mentioned above are impressive as they reveal the mystery of fidelity in understanding quantum critical phenomena. The terms in the square brackets in Eq. (9) are nothing but the dynamic structure factor of H_I. Therefore, in the original definition of fidelity, we subconsciously chose the driving term H_I as a candidate for the order parameter, though we might not think so at the time.

In order to arrive at a more computable formula, we carry out an inverse Fourier transformation and obtain

$$\chi_F = \int_0^\infty \tau[\langle \Psi_0|H_I(\tau)H_I(0)|\Psi_0\rangle - \langle \Psi_0|H_I|\Psi_0\rangle^2]d\tau, \tag{11}$$

where the first term in the square brackets can be calculated by

$$\langle \Psi_0|H_I(\tau)H_I(0)|\Psi_0\rangle = \sum_{n=0}^{\infty} \frac{\tau^n(-1)^n}{n!} e^{\tau E_0}\langle \Psi_0|H_I H^n H_I|\Psi_0\rangle. \tag{12}$$

Although fidelity is difficult to calculate from the ground-state wave functions, Eqs. (11) and (12) provide us with another practical way. In particular, Eq. (12) can be easily evaluated via the prevailing numerical techniques, say, ED and DMRG. For the ED, once the ground state is obtained, the map from one state to another new state is just a standard Lanczos step. For the DMRG, the standard algorithm involves a transformation of the Hamiltonian of a system and its environment, from a set of the old basis to a set of the new basis, which is constructed using the m largest weighted eigenstates of the reduced density matrix; or, precisely, for the system block $\bar{H}_L = O_L^\dagger H_L O_L$ and environment block $\bar{H}_R = O_R^\dagger H_R O_R$, where $O_{L(R)}$ are constructed from the m largest weighted eigenstates of the corresponding reduced density matrix. The only modification is that, in addition to $H(\lambda)$, H_I should be independently transformed in the DMRG procedure, i.e., $\bar{H}_{I,L} = O_L^\dagger H_{I,L} O_L$ and $\bar{H}_{I,R} = O_R^\dagger H_{I,R} O_R$. Once the final ground state is obtained, the mapping $|\Psi'\rangle = H_I|\Psi\rangle$ and $|\Psi'\rangle = H|\Psi\rangle$ is simply a standard step.

III. FIDELITY AND FIDELITY SUSCEPTIBILITY IN SOME MODELS

In previous works [1–6], the fidelity gives us the strong impression that it can be used to signal any phase transition. For example, in the Ising model [1,2], the fidelity collapses to zero at the critical point. From Eq. (5), such a singular behavior can be interpreted as the divergence of the fidelity susceptibility. This interpretation is consistent with that the fidelity is intrinsically based on the Landau symmetry-breaking theory. The order parameter is just the driving term in the Hamiltonian; then the divergence of the fidelity susceptibility becomes a crucial condition to signal a phase transition of Landau's type. However, this restriction also causes the fidelity to fail to identify those phase transitions that are of infinite order.

To check this point and also verify the above expressions, we now study the fidelity susceptibility of a nontrivial model in condensed matter physics, more specifically, the one-dimensional Hubbard model, where the phase transition happening at the half-filling case is of infinite order. The Hamiltonian of the Hubbard model reads

$$H = -t\sum_{\langle jl\rangle\sigma} c_{j,\sigma}^\dagger c_{l,\sigma} + U\sum_j n_{j,\uparrow}n_{j,\downarrow}, \tag{13}$$

where $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ are the creation and annihilation operators for electrons with spin σ (with $\sigma = \uparrow, \downarrow$) at site j, respectively, $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$, t is the hopping integral, and U denotes the strength of the on-site interaction. At half filling, the ground state of the Hubbard model undergoes a quantum phase transition from an ideal conductor to a Mott insulator at the point $U=0$ [13]. For simplicity, we diagonalize the Hamiltonian for a ten-site system with periodic boundary conditions using the Lanczos method, and compute fidelities with various interaction intervals and their corresponding susceptibilities. Numerical results are shown in Fig. 1. Obviously, they support our conclusion that fidelity susceptibility rather than fidelity is more crucial in the ground state. That is, the fidelity susceptibility does not depend on the value of δU, but the fidelity does. This fact makes it possible to evaluate the fidelity from the ground state $|\Psi_0(U)\rangle$ without knowledge of $|\Psi_0(U \pm \delta U/2)\rangle$.

Another interesting observation is that the fidelity susceptibility is not a maximum, nor is the fidelity a minimum, at the critical point. This fact goes somewhat beyond the physical intuition aroused by the original research motivation [2], which expects that the fidelity should be a minimum at the critical point. Although a finite-size scaling analysis (see Fig. 2) shows that the fidelity susceptibility at $U=0$ may become larger and larger as the system size increases, the divergence of the rescaled fidelity susceptibility χ_F/N [14,15] at the critical point is an unexpected phenomenon (see Fig. 3). It is because, for the half-filled Hubbard model, the phase transition at $U=0$ is of the Kosterlitz-Thouless type. In this case,

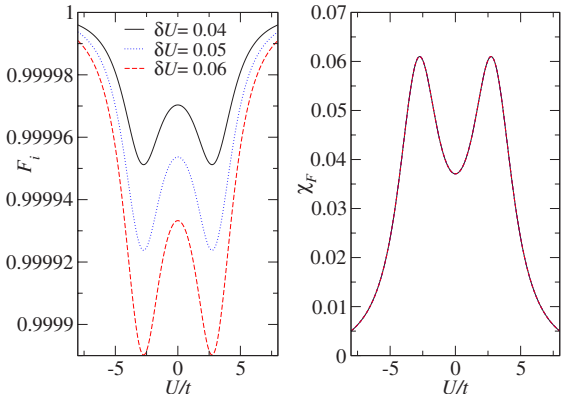

FIG. 1. (Color online) Left: Fidelity between two states separated by different $\delta U=0.04,0.05,0.06$, versus U/t of the half-filled Hubbard model with $N=L=10$ and periodic boundary conditions. Right: Fidelity susceptibility χ_F as a function of U/t, obtained from the data of the left picture. All lines in the left picture collapse to a single line.

the ground-state energy as a function of U can be expanded to any order around $U=0$, and the density-density correlation defined by the U term in the Hamiltonian (13) does not have a long-range order; thus the local order parameter for the symmetry-breaking theory is not well defined. On the other hand, if U deviates from the critical point, the scaling behavior shown in Fig. 2 manifests that the fidelity susceptibility may increase in the small-U region. However, as L increases, the trend of χ_F is still similar as in the case of $U=0$. Therefore, to find an appropriate driving term is very crucial for understanding the role of fidelity in quantum critical phenomena. For the Hubbard model, in adition to the U term, it seems be very necessary to introduce another nonlocal term for the fidelity. Nevertheless, it is still a challenging problem at present.

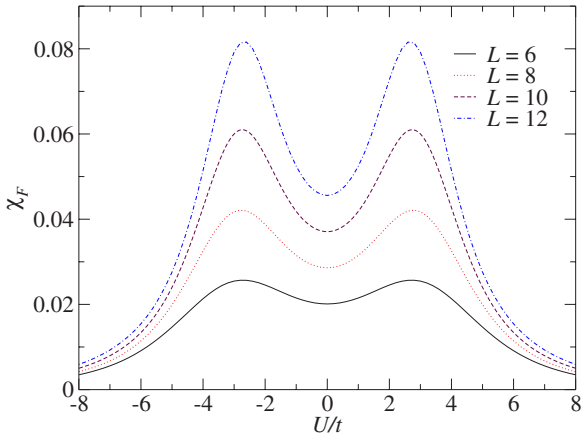

FIG. 2. (Color online) Fidelity susceptibility as a function of U/t for various system sizes. In order to avoid degeneracy in the ground state, the systems of $L=6$ and 10 are diagonalized with periodic boundary conditions, and the systems of $L=8$ and 12 with antiperiodic boundary conditions.

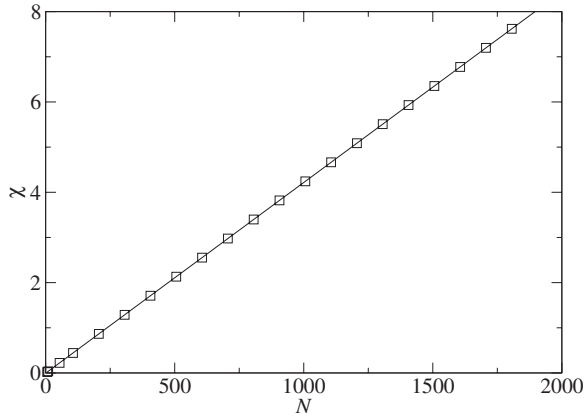

FIG. 3. Scaling behavior of the fidelity susceptibility up to 1906 sites for the half-filled Hubbard model at $U=0$. Clearly, χ/N is a constant if N is very large.

IV. MIXED-STATE FIDELITY AND THERMAL PHASE TRANSITIONS

The generalization of fidelity to finite temperatures was proposed recently. Based on the definition of fidelity between two mixed states, it has been shown that the fidelity can be expressed in terms of the partition function [4],

$$F_i(\beta,\delta)=\frac{Z(\beta)}{\sqrt{Z(\beta-\delta\beta/2)Z(\beta+\delta\beta/2)}}, \tag{14}$$

where $\beta=1/T$, and

$$Z(\beta)=\sum_n e^{-\beta E_n}=\sum_E g(E)e^{-\beta E}. \tag{15}$$

Here $g(E)$ is the density of states and can be calculated from Monte Carlo simulations [11], using, for instance, the Wang-Landau algorithm [12]. Then the fidelity susceptibility driven by temperature can be calculated as

$$\chi_F=\left.\frac{-2\ln F_i}{\delta\beta^2}\right|_{\delta\beta\to 0}=\frac{C_v}{4\beta^2}. \tag{16}$$

Similarly, if the driving term in the Hamiltonian is a Zeemann-like term, which is crucial in Landau symmetry-breaking theory, then the fidelity susceptibility is simply the magnetic susceptibility χ,

$$\chi_F=\left.\frac{-2\ln F_i}{\delta h^2}\right|_{\delta h\to 0}=\frac{\beta\chi}{4}. \tag{17}$$

Clearly, the specific heat is simply the fluctuation of the internal energy, i.e., $C_v=\beta^2(\langle E^2\rangle-\langle E\rangle^2)$, while the magnetic susceptibility is the fluctuation of the magnetization, i.e., $\chi=\beta(\langle M^2\rangle-\langle M\rangle^2)$. Thus fidelity susceptibility is just the fluctuation (structure factor) of the driving term in the Hamiltonian.

V. SUMMARY

In summary, we established a general relation between the fidelity and the structure factor of the driving term of the

Hamiltonian for both quantum and classical critical phenomena. This relation not only enables us to evaluate the fidelity easily through prevailing numerical techniques such as DMRG, ED, and Monte Carlo simulations, but also builds a straightforward connection between concepts in quantum-information theory and those in quantum many-body physics.

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