Fidelity, dynamic structure factor, and susceptibility in critical phenomena

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Motivated by the increasing research interests in the role of the fidelity in quantum critical phenomena, we establish a general relation between the fidelity and the structure factor of the driving term of the Hamiltonian through a new introduced concept: fidelity susceptibility. Our relation, as shown by some examples, makes the fidelity be easily evaluated from its susceptibility via some well developed techniques, such as density matrix renormalization group for the ground state, and Monte-Carlo simulation for the thermal equilibrium state.

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Quite recently, an increasing interest [1, 2, 3, 4, 5] has been drawn in the role of fidelity, a concept borrowed from the quantum information theory [6], in quantum critical phenomena [7]. The common motivation behind these studies is straightforward. Since the fidelity is a measure of the state-state distance, the dramatic change of the structure of the ground state around the quantum critical point should result in a large distance between two ground states, which are on both sides of the critical point. For example, in the one-dimensional XY model, the fidelity shows a narrow downward peak at the phase transition point [2]. Similar properties were also found in fermionic [3] and bosonic systems [5]. Since the fidelity is a pure quantum information concept, these works actually built a connection between the quantum information theory and condensed matter physics.

However, except for some special models, such as one-dimensional XY model and Dicke model[1, 2], evaluating the fidelity from the ground-state wavefunction is tedious. Therefore, a neater and easier strategy based on some well developed techniques is of great importance for the extensive application of the fidelity to the critical phenomena. For this purpose, we introduce the concept of fidelity susceptibility which defines the response of fidelity to the driving parameter in the Hamiltonian. At zero temperature, we show that the fidelity susceptibility actually defines the response of fidelity to the driving parameter in the Hamiltonian. Here $H_I$ is the driving Hamiltonian and $\lambda$ denotes its strength. Then the eigenstates $|\Psi_n(\lambda)\rangle$ satisfy $H(\lambda)|\Psi_n(\lambda)\rangle = E_n(\lambda)|\Psi_n(\lambda)\rangle$ defines a set of orthogonal and complete basis of the Hilbert space. Here we restrict ourselves to the phase transition which is not induced by the ground-state level-crossing. That means that the ground state of the Hamiltonian is non-degenerate for a finite system. We next change $\lambda \rightarrow \lambda + \delta \lambda$ where $\delta \lambda$ is so small that the perturbation theory is applicable. Up to the first-order perturbation, the ground state becomes

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

where

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

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

$$F_1(\lambda, \delta) = |\langle \Psi_0(\lambda)|\Psi_0(\lambda + \delta)\rangle|.$$

Therefore, to the lowest order, we have

$$\frac{1}{F_1^2} = 1 + \delta \lambda^2 \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda)|H_I|\Psi_0(\lambda)\rangle|^2}{|E_n(\lambda) - E_0(\lambda)|^2}$$

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

$$\chi_F \equiv \lim_{\delta \lambda \rightarrow 0} -\frac{2 \ln F_1}{\delta \lambda^2}.$$
From Eq. (5), it takes the form

$$\chi_F(\lambda) = \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda) | H_I | \Psi_0(\lambda) \rangle|^2}{|E_n(\lambda) - E_0(\lambda)|^2}$$  \hspace{1cm} (7)$$

in the ground state. Here we would like to point out that, though the above procedure is based on the perturbation theory, the fidelity susceptibility only depends the spectra of the Hamiltonian $H(\lambda)$ and the hoping matrix $H_{10}$. Unfortunately, Eq. (7) is almost not computable except for some very small system which are usually far away from the scaling region. In order to overcome this difficulty, it is then necessary to consider the time evolution of the system. For simplicity, we omit the parameter $\lambda$ in the following expression, and define the dynamic fidelity susceptibility as

$$\chi_F(\omega) = \sum_{n \neq 0} \frac{|\langle \Psi_n | H_I | \Psi_0 \rangle|^2}{|E_n - E_0|^2 + \omega^2}$$  \hspace{1cm} (8)$$

Make a Fourier transformation and take a derivative, we then obtain

$$\frac{\partial \chi_F(\tau)}{\partial \tau} = -\pi \left[ \langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2 \right] \theta(\tau) + \pi \left[ \langle \Psi_0 | H_I(0) H_I(\tau) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2 \right] \theta(-\tau).$$  \hspace{1cm} (9)$$

where $\tau$ is imaginary time, and

$$H_I(\tau) = e^{H(\lambda)\tau} H_I e^{-H(\lambda)\tau}$$  \hspace{1cm} (10)$$

The above two equations are very impressive. They reveal the mysterious veiling of the fidelity for the understanding of quantum critical phenomena. The term in the bracket in Eq. (9) is nothing but the dynamic structure factor of $H_I$. Therefore, in the original definition of the fidelity, we subconsciously choose the driving term $H_I$ as a candidate of the order parameter, though we may do not think so at that time. From this point of view, we would like to emphasize that the study on the role of fidelity in critical phenomena still does not go beyond the traditional Landau’s symmetry-breaking theory.

In order to have a more computable formula, we make an inverse Fourier transformation and obtain

$$\chi_F = \int \tau \left[ \langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2 \right] d\tau$$  \hspace{1cm} (11)$$

where the first term in the bracket can be calculated by

$$\langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle = \sum_n \frac{\tau^n (-1)^n}{n!} e^{iE_0} \langle \Psi_0 | H_I H^n H_I | \Psi_0 \rangle.$$  \hspace{1cm} (12)$$

Therefore, though the fidelity is difficult to be calculated from the ground-state wavefunctions, Eq. (11) and (12) actually provide us another computable way. Especially, Eq. (12) can be easily evaluated via the prevailing numerical techniques. Here let us take the DMRG as an example. The standard DMRG algorithm includes a transformation of the Hamiltonian of the system and environment from a set of old basis to another set of new basis spanned by the largely weighted eigenstates of the reduced density matrix. The only modification is that, in addition to $H(\lambda)$, $H_I$ should be individually transformed in the DMRG procedure. Then once the final ground-state is obtained, the mapping $|\Psi'\rangle = H_I |\Psi\rangle$ and $|\Psi'\rangle = H |\Psi\rangle$ is simply the standard step in the Lanczos method.

To check the correctness of the above expressions, we now study the fidelity susceptibility in a non-trivial dimensional Hubbard model, whose Hamiltonian reads

$$H = -t \sum_{\langle j \rangle, \sigma} c_{j,\sigma}^\dagger c_{j,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow},$$  \hspace{1cm} (13)$$

where $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$, $\sigma = \uparrow, \downarrow$ are creation and annihilation operators for electrons with spin $\sigma$ at site $j$ respectively.

![FIG. 1: The fidelity susceptibility (LEFT) and fidelity (RIGHT) as a function of $U$ in the ground state of half-filled Hubbard model with $N = L = 6$ and $N = L = 10$. In the right picture, square points ($L = 6$) and circle points ($L = 10$) are obtained from the wavefunction overlap with $\delta U = 0.2$ (Eq. (3)), while the two lines from the data in the left picture with the same $\delta U = 0.2$.](image)
The fidelity susceptibility $\chi_F$ is more crucial in the ground state. Another conclusion that the fidelity susceptibility rather than the fidelity and its susceptibility via different ways. The numerical results are shown in Fig. 1, and clearly support our observation that the fidelity can describe all kinds of phase transition. Moreover, we establish a general relation between the fidelity susceptibility rather than fidelity in the thermal phase transition, we take two-dimensional Ising model defined on a square lattice as an example. The Hamiltonian reads

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z,$$

where the sum is over all pairs of nearest-neighbor sites $i$ and $j$, and the coupling is set to unit for simplicity. We use the Wang-Landau algorithm [11] to compute the density of state in Eq. (15). Then the fidelity susceptibility driven by the temperature can be calculated as

$$\chi_F = -\frac{2\ln F_i}{\delta F^2} \bigg|_{\delta F=0} = \frac{C_v}{4\beta^2},$$

Similarly, if the driving term in the Hamiltonian is the Zeemann-like term, which is crucial in the Landau’s symmetry-broken theory, then the fidelity susceptibility is the magnetic susceptibility $\chi$,

$$\chi_F = -\frac{2\ln F_i}{\delta h^2} \bigg|_{\delta h=0} = \frac{\beta \chi}{4}. \quad (17)$$

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

To confirm our understandings and show the more important role of the fidelity susceptibility rather than fidelity in the thermal phase transition, we take two-dimensional Ising model defined on a square lattice as an example. The Hamiltonian reads

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z,$$