

Fidelity susceptibility, scaling, and universality in quantum critical phenomena

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We study fidelity susceptibility in the one-dimensional asymmetric Hubbard model and show that the fidelity susceptibility can be used to identify the universality class of the quantum phase transitions in this model. The Kosterlitz–Thouless-type transition occurred at half-filling and the Landau transition away from half-filling can be discriminated from distinct critical exponents of the fidelity susceptibility.

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I. INTRODUCTION

Quantum phase transitions (QPTs) of a many-body system at zero temperature are characterized by the change of the ground-state properties as model parameter λ in the system Hamiltonian $H(\lambda)$ is varied across the transition point λ_c .¹ This primary observation motivates people to explore the role of fidelity, a concept emerging from quantum information theory,² in critical phenomena.^{3,4} Since the fidelity measures the similarity between states, the change in the ground-state structure around the quantum critical point should result in a dramatic change in the fidelity across the critical point. Such a fascinating prospect was first demonstrated in the one-dimensional (1D) XY model, where the fidelity shows a narrow trough at the phase-transition point.^{3,4} Afterward, the fidelity was used to characterize the QPTs in fermionic⁵ and bosonic systems.⁶ So these works established another connection between quantum information theory and condensed-matter physics, in addition to the recent studies on the role of the entanglement in QPTs.^{7–12} The motivation for exploring the role of the fidelity in QPTs is obvious: since the fidelity is purely a quantum information concept, where no *a priori* knowledge of the order parameter and the change of symmetry in the system is assumed, it would be a great advantage if one can use it to characterize the QPTs.^{13–18}

The fidelity actually reflects the response of the ground state to the change of the QPT driving parameter. Recently, Zanardi *et al.*¹⁴ introduced the Riemannian metric tensor inherited from the parameter space to denote the leading term in the fidelity, and argued that the singularity of this metric corresponds to the QPTs. At the same time, You *et al.*¹⁵ introduced another concept, the so-called fidelity susceptibility (FS), and established a general relation between the leading term in the fidelity and the structure factor of the driving term in the Hamiltonian. This relation implies that the fidelity may not have a singular behavior in transitions of infinite order, such as the Kosterlitz–Thouless (KT) phase transition.¹⁹

In this paper, we show that the FS can be used to characterize the universality class²⁰ in quantum critical phenomena by studying the FS in two quantum many-body models. First we perform a scaling analysis of the FS for a general system and show the critical exponent of the FS can be used to describe the universality class of the quantum phase transitions, as illustrated by the well-studied 1D transverse-field

Ising model. Then we focus on the critical behavior of the FS in the 1D asymmetric Hubbard model (AHM).²¹ Since the AHM can be used to describe a mixture of two species of fermionic atoms in optical lattices, which has been realized by recent experiments on the cold atoms,²² so the model itself is of current research interest,^{23–28} and its universality class, to the best of our knowledge, has not been discussed. By analyzing the FS, we obtained the critical point and corresponding exponents in the 1D AHM, and found that the QPTs occurred at various band fillings can be characterized by critical exponents. For example, the system size scaling exponent of the FS is found to be 5.3 away from half-filling (e.g., $n=2/3$) and 1 at half-filling. We would like to emphasize that the critical exponents here are obtained without any knowledge of the symmetry of the system.

This paper is organized as follows: In Sec. II, we discuss scaling and critical properties of the FS in a general quantum phase transition. In Sec. III, we study numerically the FS in the ground state of the 1D AHM for both cases of $n=2/3$ and $n=1$. Finally, our conclusions are given in Sec. IV.

II. SCALING ANALYSIS OF THE FIDELITY SUSCEPTIBILITY

To begin with, we consider a general Hamiltonian of quantum many-body systems,

$$H(\lambda) = H_0 + \lambda H_\lambda, \quad (1)$$

where H_λ is the part of the Hamiltonian that drives QPTs with the strength λ . Following Ref. 4, the fidelity is defined as the overlap between two ground states $|\Psi_0(\lambda)\rangle$ and $|\Psi_0(\lambda + \delta\lambda)\rangle$, i.e.,

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

The FS is just the most relevant term in the fidelity,

$$\chi_{F(\lambda)}(\lambda) = \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda) | H_\lambda | \Psi_0(\lambda) \rangle|^2}{[E_n(\lambda) - E_0(\lambda)]^2}, \quad (3)$$

where $|\Psi_n(\lambda)\rangle$ satisfies $H(\lambda)|\Psi_n(\lambda)\rangle = E_n(\lambda)|\Psi_n(\lambda)\rangle$ and defines a set of orthonormal basis in the Hilbert space. The FS is mathematically related to the structure factor of the driving term H_λ ,¹⁵ which denotes the fluctuation caused by the driving parameter λ . For example, by extending the fidelity to the thermal state,¹³ the FS is simply the specific heat or the

magnetic susceptibility^{14,15} if we choose the driving parameter as temperature or magnetic field, respectively. Therefore, the singular behavior of the FS corresponds to a phase transition. However, this picture might not be true for the KT-type transition. For the KT transition, despite of the vanishing energy gap, there is still no singularity in the FS as matrix elements $\langle \Psi_n(\lambda) | H_I | \Psi_0(\lambda) \rangle$ also vanish at the same time. The appearance of the power-law decay behavior reveals a stronger fluctuation around the critical point. Thus the FS, by its definition, might reach a maximum around the critical point, although the maximum point is not necessary right at the critical point, as has been observed in the 1D Hubbard model.¹⁵

Similar to other approaches describing phase transitions, we can also extract critical exponents from the FS. In the most cases, the FS usually depends linearly on the system size, i.e.,

$$\chi_{F(\lambda)}(\lambda) \propto L, \quad (4)$$

in the noncritical region. Then the average FS $\chi_{F(\lambda)}(\lambda)/L$, as an intensive quantity in the thermodynamic limit, scales like

$$\frac{\chi_{F(\lambda)}(\lambda)}{L} \propto \frac{1}{|\lambda_c - \lambda|^\alpha}, \quad (5)$$

around the critical point λ_c with α being corresponding exponent. There are rare cases (such as the FS in the Lipkin–Meshkov–Glick model²⁹) that $\chi_{F(\lambda)}(\lambda)$ is not a linear function of L , then the left term in Eq. (5) can be replaced by a general $\chi_{F(\lambda)}(\lambda)/L^{\mu'}$, where μ' is the size exponent of the FS in the noncritical region. On the other hand, if the average FS around the critical point shows a peak for a finite system, its maximum point at λ_{\max} scales like

$$\chi_{F(\lambda)}(\lambda = \lambda_{\max}) \propto L^\mu. \quad (6)$$

So we introduce the following function to include the above two asymptotic behaviors:

$$\frac{\chi_{F(\lambda)}(\lambda)}{L} = \frac{A}{L^{-\mu+1} + B(\lambda - \lambda_{\max})^\alpha}, \quad (7)$$

where A is a constant, B is a nonzero function of λ , and both of them are independent of the system size. According to Eq. (7), the rescaled FS is a universal function of the rescaled driving parameter $L^\nu(\lambda - \lambda_{\max})$, i.e.,

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

where ν is the critical exponent of the correlation length and $f(x)$ is an even function of x around the zero point. Combining Eqs. (5)–(8), we can find a relation among the three exponents, that is,

$$\alpha = \frac{\mu - 1}{\nu}. \quad (9)$$

As a direct demonstration, we revisit the well-studied 1D transverse-field Ising model, whose Hamiltonian reads

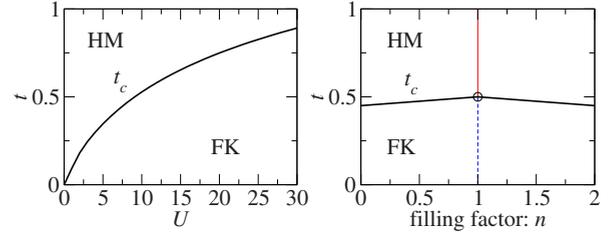


FIG. 1. (Color online) The schematic phase diagram of the AHM. Left: The phase diagram defined on the U - t plane, which shows a KT transition at half-filling and the Landau transition away from half-filling. Right: The phase diagram defined on the n - t plane, in which the transition along the middle line is of KT type and the thin solid lines at both sides are of Landau type. The phase diagram has a mirror symmetry about the line $n=1$ due to the particle-hole symmetry in the model.

$$H_{\text{Ising}} = \sum_j [\sigma_j^z \sigma_{j+1}^z + \lambda \sigma_j^x], \quad (10)$$

where σ is the Pauli matrix. Obtained in Ref. 4 were $\mu=2$ and $\mu'=1$, and $\nu=1$ is known, so $\alpha=1$; Eq. (9) is satisfied. Thus, the relation between the FS and the Landau's symmetry-breaking theory (LSBT) is straightforward: the universality classes could be identified by the critical exponents of the FS.

III. FIDELITY SUSCEPTIBILITY IN THE ONE-DIMENSIONAL ASYMMETRIC HUBBARD MODEL

We now turn to the 1D AHM, whose Hamiltonian reads

$$H_{\text{AHM}} = - \sum_{j=1}^L \sum_{\delta=\pm 1} \sum_{\sigma} t_{\sigma} c_{j,\sigma}^{\dagger} c_{j+\delta,\sigma} + U \sum_{j=1}^L n_{j,\uparrow} n_{j,\downarrow}, \quad (11)$$

where $c_{j,\sigma}^{\dagger}$ and $c_{j,\sigma}$, $\sigma = \uparrow, \downarrow$ are creation and annihilation operators for fermionic atoms with spin σ at site j , respectively, $n_{\sigma} = c_{\sigma}^{\dagger} c_{\sigma}$, t_{σ} is σ -dependent hopping integral, and U denotes the strength of on-site interaction. The Hamiltonian (11) has $U(1) \otimes U(1)$ symmetry for general t_{σ} , and the atom numbers $N_{\uparrow} = \sum_j n_{j,\uparrow}$ and $N_{\downarrow} = \sum_j n_{j,\downarrow}$ are conserved. The total number of atoms is given by $N = N_{\uparrow} + N_{\downarrow}$ and the filling factor is $n = N/L$. For simplicity, we reset $t = t_{\downarrow}/t_{\uparrow}$ and U to be U/t_{\uparrow} .

The phase diagram of the AHM has been extensively studied in Refs. 21, 27, and 28. A schematic phase diagram of the AHM is shown in Fig. 1, whose qualitative features can be understood from its two limiting cases, the Falicov–Kimball (FK) model region^{30,31} ($t_{\downarrow}=0$) and the Hubbard model region³² ($t_{\downarrow}=t_{\uparrow}$). We should point out that band filling plays a distinct role in the AHM. Away from the half-filling, the system is an ideal conductor and in the density wave state in the Hubbard region, but in a phase separation state in the FK region. For the latter, the translational symmetry is broken and the phase transition is of Landau type.^{27,28} While at half-filling, the ground state is a spin-density wave in both the Hubbard region and the FK region. The difference is that in the Hubbard region, the system renormalizes to the Heisenberg fixed point, while in the FK region, it renormalizes to the Ising fixed point. In the large U limit, the model

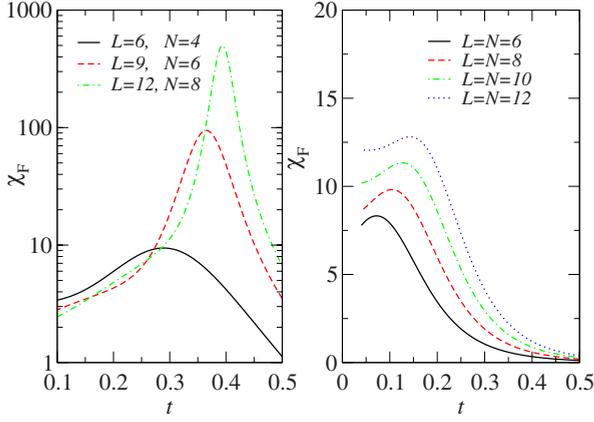


FIG. 2. (Color online) The scaling behavior of the FS as a function of t for the cases of $n=2/3$ (left) and $n=1$ (right). Here $U=30$.

can be approximated by the XXZ model,²¹ i.e.,

$$H = J \sum_{j=1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z), \quad (12)$$

where

$$J = \frac{t_{\uparrow} t_{\downarrow}}{U}, \quad \Delta = \frac{t_{\uparrow}^2 + t_{\downarrow}^2}{2t_{\uparrow} t_{\downarrow}}. \quad (13)$$

For the XXZ model, the exact solution has already been obtained by the Bethe-ansatz method.³³ Its ground-state energy can be expanded to an arbitrary order of Δ , and the spin-spin correlation function around the critical point is of power-law decay. Therefore, the QPT occurred between these two regions is of KT type.²¹

In order to quantify the change in the ground state during the evolution of t , we define the fidelity of the 1D AHM as

$$F(t, \delta t) = |\langle \Psi(t) | \Psi(t + \delta t) \rangle|. \quad (14)$$

The corresponding FS is

$$\chi_{F(t)}(t) = -2 \lim_{\delta t \rightarrow 0} \frac{\ln F(t, \delta t)}{\delta t^2}. \quad (15)$$

We study $\chi_{F(t)}$ in two special cases, away from half-filling ($n=2/3$) and the half-filling ($n=1$), with interaction $U=30$. The numerical results of different system sizes obtained from exact diagonalization are presented in Fig. 2, where boundary conditions were carefully chosen so to avoid ground-state-level crossing induced by finite lattice size effects. For both cases, the FS reaches a maximum point at a certain position t_{\max} . The difference is that for $n=2/3$, $\chi_{F(t)}(t=t_{\max})$ diverges dramatically with increasing system size, while for $n=1$, $\chi_{F(t)}(t=t_{\max}) \propto L$. The former behavior clearly shows a Landau-type transition and the latter a KT-type transition.

To study the critical behavior of the FS around the transition point at $n=2/3$, we perform finite-size scaling analysis. According to the scaling ansatz³⁴ and conclusions of Sec. II, we show the rescaled FS as a function of rescaled t in Fig. 3 for the case of $U=30$, in which numerical results obtained from various system sizes fall onto a single line. The maxi-

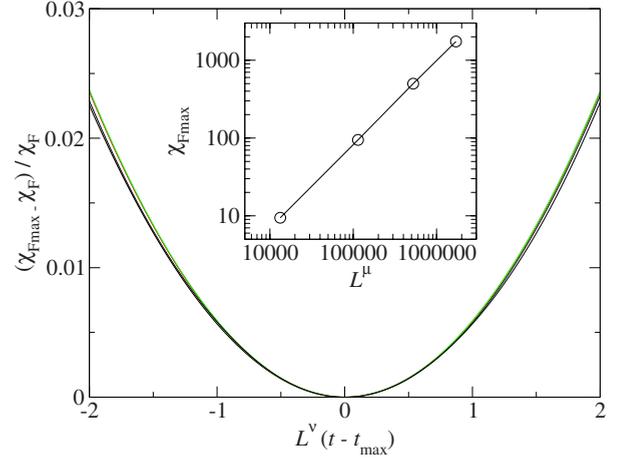


FIG. 3. (Color online) The finite-size scaling analysis is performed for the case of power-law divergence at $U=30$, $n=2/3$, and system sizes $L=6, 9, 12, 15$. The FS shows to be a function of $L^\nu(t-t_{\max})$ only, with the critical exponent $\nu \approx 2.65$. The inset exhibits the scaling behavior of $\chi_{F(t=t_{\max})}$. The straight line is of slope 1 in the logarithmic scale and $\mu \approx 5.3$. (See text for details.)

mum value of the FS diverges with increasing system size as: $\chi_{F(t)}(t=t_{\max}) \propto L^\mu$. For the 1D AHM, the FS should be averaged over the system size, so $\chi_{F(t)}(t=t_{\max})/L \propto L^{\mu-1}$. Thus the exponent ν together with μ determines the critical exponent α in Eq. (5). For the present case, we find $\nu \approx 2.65$ and $\mu \approx 5.3$; hence $\alpha = (\mu - 1)/\nu \approx 1.6$, which clearly differs from the Ising model. For the Ising model of Eq. (10), only Z_2 symmetry is broken when the phase transition occurs, while in the AHM, the translational symmetry is broken in the phase separation region, so they belong to different universality classes. The critical t_c can be obtained by $1/L$ extrapolation. In the left plot of Fig. 4, we show the scaling behavior of the t_{\max} . The critical points are found to be $t_c \approx 0.294, 0.402, 0.459$ for $U=10, 20, 30$, respectively.

At half-filling $n=1$, the KT transition occurs. The corresponding finite scaling analysis for the case of $U=30$ is presented in Fig. 5. The maximum point of the FS is proportional to the system length. This is consistent with our

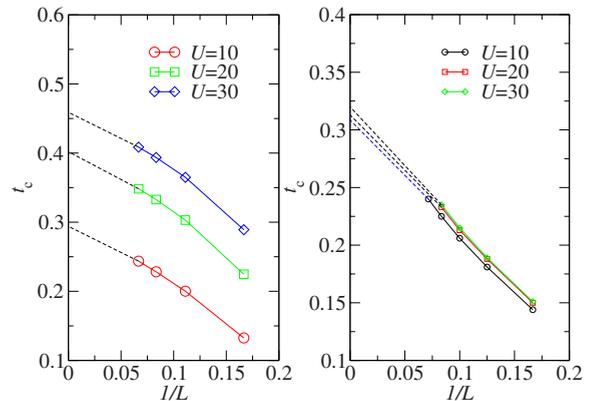


FIG. 4. (Color online) The critical t_c are evaluated from $1/L$ extrapolation for $n=2/3$ (left) and $n=1$ (right), respectively. The dashed lines correspond to the expected behavior for $1/L \rightarrow 0$ according to linear fitting.

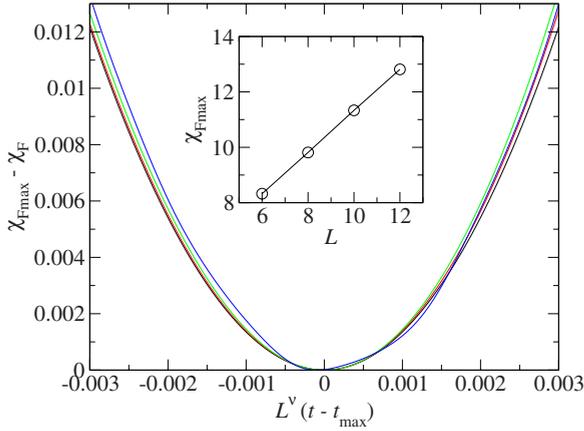


FIG. 5. (Color online) Similar finite-size scaling is performed for the case of KT transition with various system sizes $L = 6, 8, 10, 12$ at $n=1$ and $U=30$. The FS shows to be a function of $L^\nu(t-t_{\max})$ only, with the critical exponent $\nu \approx -0.25$. The inset exhibits the scaling behavior of $\chi_F(t=t_{\max})$. (See text for details.)

mentioned understanding. Again, the rescaled FS for various system sizes fall onto a single line, which is a function of $L^\nu(t-t_{\max})$ with critical exponent $\nu = -1/4$. We find that around the maximum point t_{\max} the FS behaviors as

$$\chi_{F(t)} \approx 3.86 + 0.75L + 1350L^{-1/2}(t-t_{\max})^2, \quad (16)$$

approximately. Referring to Eq. (5), we have $\alpha=0$. As expected, there is no singularity in $\chi_{F(t)}(t)$. Due to the system size exponent $-1/2$ in the last term of Eq. (16), the maximum behavior becomes weak with the increasing system size, as is also shown in Fig. 2. The relative larger FS in the FK region can be understood from its effective model, i.e., the XXZ model, in which the transition from quantum fluctuation (Hubbard region) to Ising order (FK region) occurs at the isotropic point. The transition is of KT type, and the correlation function $\langle \sigma_j^z \sigma_{j+r}^z \rangle$ is of exponential decay in the Hubbard region and of power-law decay in the FK region. The FS, as an indicator of the fluctuation of the anisotropic term in the XXZ model, should have a large value in the FK region.

In analogy with the KT transition that occurred in the quantum XY model,³⁵ we guess that the very steep decreasing point of the FS in Fig. 2 is more closer to the exact critical point. Therefore, we also take the first-order derivative of the FS with respect to t and perform $1/L$ finite scaling analysis for the minimum point of $d\chi_{F(t)}(t)/dt$. Numerical data are shown in the right plot of Fig. 4. In the thermodynamic limit, we find that $t_c \approx 0.308, 0.313, 0.317$ for $U = 10, 20, 30$, respectively. The results are close to those ob-

tained by the density-matrix renormalization-group method,²¹ which suggested that the critical point locate in the range $[0.3, 0.4]$ for the case of $U=10$.

Similar analysis can be applied to other fillings. The power-law divergence of the FS $\chi_{F(t)}(t)/L$ always exists for any fillings other than the half-filling ($n=1$). Since the AHM possess particle-hole symmetry, so the FS takes the same value for band fillings n and $2-n$ ($n < 2$) and the phase diagram in the $n-t$ plan has a mirror symmetry about the line $n=1$. Take into account the fact that even a single hole doping away from half-filling leads to the instability of the density wave state in the infinite U limit,²⁷ we conclude that the KT transition occurs only at half-filling; so the transition point at $n=1$ is expected to be a quar-critical point on the phase diagram, and the behavior of FS signals the transition type along the critical lines.

IV. CONCLUSION

In conclusion, we have shown that the FS, as the leading term in the fidelity between two ground states at different parameter space, can be used to characterize the universality class in quantum critical phenomena. Since the FS is related to the structure factor of the phase-transition driving term in the Hamiltonian, it is linked up to the LSBT straightforwardly, so the critical exponent associated with FS is a natural candidate for the classification of the universality. We elucidated this point by the simple QPT that occurred in the 1D transverse-field Ising model. On the other hand, despite no singularity appearing in the FS when crossing a KT transition point, the stronger fluctuation might make the FS reach a maximum near the critical point. The nonsingular behavior of the FS in the KT transition is also pointed out in later investigations.³⁶ In connection with recent progress in cold atom systems, we studied the FS in the 1D AHM and showed that the FS can help us to identify both types of phase transition in this model. The critical exponent α for the Landau-type transition is calculated with finite-size scaling analysis and is found to be 1.6 for $n=2/3$ filling. While for the KT transition, $\alpha=0$ for $n=1$ in the thermodynamic limit, and FS scales linearly with system size.

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