Fidelity susceptibility, scaling, and universality in quantum critical phenomena

Shi-Jian Gu,1, 2 Ho-Man Kwok,1 Wen-Qiang Ning,1, 2 and Hai-Qing Lin1

1Department of Physics and ITP, The Chinese University of Hong Kong, Hong Kong, China
2Department of Physics, Fudan University, Shanghai 200433, China

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We study fidelity susceptibility in one-dimensional asymmetric Hubbard model, and show that the critical exponents are found to be 0 and 2 for cases of half-filling and away from half-filling respectively.

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Quantum phase transitions (QPTs) at zero temperature are characterized by the significant change in the ground state of a many-body system as a parameter \( \lambda \) in the system Hamiltonian \( H(\lambda) \) is varied across a point \( \lambda = 0 \). This primary observation enlightens people to explore the role of fidelity, a concept emerging from quantum information theory [2], in the critical phenomena [3, 4]. Since fidelity is a measure of similarity between states, a dramatic change in the structure of the ground state around a quantum critical point should result in a great difference between the two ground states on the both sides of the critical point. Such a fascinating prospect was firstly confirmed in the 1D XY model where the fidelity shows a narrow trough at the phase transition point [2, 3]. From then on, the fidelity was further used to characterize the QPTs in fermionic [5] and bosonic systems [6]. As fidelity is purely a quantum information concept, an obvious advantage is that it can be a promising candidate to characterize the QPTs [7, 8, 9, 10, 11, 12] because no a priori knowledge of the order parameter and the symmetry of the system is needed. Therefore, these works established another connection between quantum information theory and condensed matter physics, in addition to the recent studies on entanglement in QPTs [13, 14, 15, 16, 17, 18].

The fidelity actually reflects the response of the ground state to a small change of the driving parameter. Zanardi et al. introduced the Riemannian metric tensor [8] inherited from the parameter space to denote the leading term in the fidelity, and argued that the singularity of this metric is in correspondence with the QPTs. While You et al. introduced another concept, so-called fidelity susceptibility (FS) [9], 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 singular behavior in those transitions of infinite order, such as Kosterlitz-Thouless (KT) transitions [19].

In this work, we study the FS in 1D asymmetric Hubbard model (AHM) [21], and show that the FS can be used to characterize the universality class [20] in quantum critical phenomena. The intrinsic relation between the FS and the Landau’s symmetry-breaking theory (LSBT) is firstly clarified by a simple QPT occurred in a well-studied 1D transverse-field Ising model. Then we mainly focus on the critical behavior of the FS in the 1D AHM. Since the AHM can be used to describe a mixture of two species of fermionic atoms in an optical lattice, which is able to be realized by recent experiments on the cold atoms [22], the model itself is of current research interest [23, 24, 25, 26, 27, 28]. We find that the critical exponents of the FS take the value of 0 and 2 for cases of half-filling \((n = 1)\) and away from half-filling \((n = 2/3)\) respectively.

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

\[
H(\lambda, h) = H_0 + \lambda H_I + h M,
\]

where \( H_I \) is the driving Hamiltonian with the strength \( \lambda \), and \( M \) is a potential order parameter and \( h \) is the corresponding external field. Without loss of generality, we first set \( h = 0 \). Following Ref. [4], the fidelity is defined as the overlap between two ground states \( |\Psi_0(\lambda)\rangle \) and \( |\Psi_0(\lambda + \delta \lambda)\rangle \), that is

\[
F(\lambda, \delta \lambda) = |\langle \Psi_0(\lambda) | \Psi_0(\lambda + \delta \lambda) \rangle|.
\]

Then the FS is just the most relevant term in the fidelity, and mathematically is related to the structure factor of the driving term \( H_I \), which denotes the fluctuation caused by the driving parameter. For example, if we extend the fidelity to the thermal state \( T \), the FS is just the specific heat or the magnetic susceptibility \([8, 9]\) if we choose the driving parameter as temperature or magnetic field respectively.

Compared with ordinary phase transitions, we can also extract two exponents (denoted as \( \alpha, \gamma \)) from the FS in quantum critical phenomena if we choose the driving parameter as \( \lambda \) and \( h \) (if the order parameter is known) respectively (Here, the only condition is that the QPT should belong to the type of Landau’s transition, otherwise \( \alpha = 0 \) and \( \gamma \) is not well defined). Then the fidelity susceptibilities driven by two terms in the Hamiltonian
scale like
\[
\frac{\chi_{F(\lambda)}(\lambda)}{N} \propto \frac{1}{|\lambda_c - \lambda|^\alpha}, \quad \frac{\chi_{F(h=0)}(\lambda)}{N} \propto \frac{1}{|\lambda_c - \lambda|^\gamma},
\]
respectively, around the critical point \(\lambda_c\) in the thermodynamic limit. As a simple application, we take the well-studied model, i.e. 1D transverse-field Ising model, as an example,
\[
H_{\text{Ising}} = \sum_j [\sigma_j^x \sigma_{j+1}^x + \lambda \sigma_j^z + h \sigma_j^z],
\]
where \(\sigma\) is Pauli matrix. In Ref. \[4\], it was obtained \(\alpha = 1\). On the other hand, if we consider \(h\) as the driving parameter, we find \(\beta = 1/8\) of the order parameter \(\sigma^z\), we then have \(\alpha + 2\beta + \gamma = 3\), which is slightly different from the usual \(\alpha + 2\beta + \gamma = 2\) in 2D Ising model. We interpret this difference as one more differentiation is made in the FS of the ground state than the specific heat at finite temperatures. That is, the FS is related to the second order derivative of the ground state energy with respect to the driving parameter \[3\], while for the specific heat, it is simply \(dE(T)/dT\) where \(E(T)\) is the internal energy. Therefore, the phase transition here still belongs to the same universality class of the 2D Ising model. As a brief conclusion, the relation between the FS and the LSBT is straightforward. Once the driving term and order parameter are given, the universality classes are simply described by the critical exponents of FS.

The LSBT is established on the order parameter, whose non-vanishing behavior results from the broken symmetry and long-range order. For KT transitions, both broken symmetry and long-range order are absent, hence no local order parameter is concerned. Consider again the original definition of the FS, i.e.
\[
\chi_F(\lambda) = \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda) | H_j | \Psi_0(\lambda) \rangle|^2}{|E_n(\lambda) - E_0(\lambda)|^2},
\]
where \(\langle \Psi_n(\lambda) | H_j | \Psi_0(\lambda) \rangle\) satisfies \(H(\lambda)|\Psi_n(\lambda)\rangle = E_n|\Psi_n(\lambda)\rangle\) and defines a set of orthogonal complete basis in the Hilbert space. For the KT transition, despite of the vanishing energy gap, there is still no singularity in the FS as matrix elements \(\langle \Psi_n(\lambda) | H_j | \Psi_0(\lambda) \rangle\) also vanish at the same time. However, the appearance of the power-law decay behavior describes the stronger fluctuation around the critical point. This point directly leads to that the FS, which also denotes the fluctuation of the driving term, might reach a maximum near the critical point, though the maximum point might not be the critical point, as has been observed in the 1D Hubbard model [9].

To confirm this physical intuition, we now focus on the 1D AHM, whose Hamiltonian reads
\[
H_{\text{AHM}} = -\sum_{j=1}^{L} \sum_{\delta = \pm 1} t_{\sigma} c_{j,\sigma}^\dagger c_{j+\delta,\sigma} + U \sum_{j=1}^{L} n_{j,\uparrow} n_{j,\downarrow},
\]
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, \(n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}\), \(t_{\sigma}\) is \(\sigma\)-dependent hoping integral, and \(U\) denotes the strength of on-site interaction. In this model, the Hamiltonian has \(U(1) \otimes U(1)\) symmetry for general \(t_{\sigma}\), and the atoms number \(N_\uparrow = \sum_j n_{j,\uparrow}, N_\downarrow = \sum_j n_{j,\downarrow}\) are conserved respectively. 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 \(t_j = t/\sqrt{L}\), and \(U\) to be \(U/t_j\).

The schematic phase diagram of the AHM is shown in Fig. 1 which can be understood from its two limiting cases, the Hubbard model \[30\] \((t_j = t_1)\) and the Falicov-Kimball (FK) model \[31, 32\] \((t_j = 0)\). At half-filling, both the Hubbard model and the FK model are in a spin-density-wave state. The difference is that in the Hubbard region, the system renormalizes to the Heisenberg fixed point, while in the FK region, it belongs to the Ising fixed point. The QPT occurred between these two classes belongs to the KT type in the 1D system because the correlation function at both side is of power-law decay \[21\] and no local order parameter is well defined. While away from half filling, the system becomes an ideal conductor and is in the state of density wave in the Hubbard region, but it is in a phase separation in the FK region. In the phase separation region, the translational symmetry is broken, and the down-spin electrons congregate together; then \(\langle n_{\downarrow} \rangle\) plays a role of the order parameter. So the phase transition is of Landau’s type \[27, 28\].

In order to quantify the change of the ground state during the evolution of \(t\), we define the fidelity as \(F(t, \delta t) = |\langle \Psi(t) | \Psi(t + \delta t) \rangle|\). The corresponding FS is \(\chi_{F(t)}(t) = -2 \lim_{\delta t \to 0} \ln F(t, \delta t)/\delta t^2\). To avoid the ground state level crossing, we choose the periodic or antiperiodic boundary conditions for systems with \(4L + 2\) or \(4L\) electrons respectively. We first look at two special cases, i.e. the FS at half-filling \((n = 1)\) and away from half-filling \((n = 2/3)\), and both with a given interaction \(U = 10\). The numerical results of different system sizes are presented in Fig. 2. For both cases, the
The finite size scaling analysis is needed. According to the definition of the critical exponents in Eq. (3), we introduce the following scaling behavior for the FS:

$$\chi_F(t, L) = \frac{A}{L^{-\nu} + B(t - t_{\text{max}})^\alpha}.$$  \hspace{1cm} (7)

where $A, B$ are constants independent of $L$ and $t$. Such a finite size scaling leads to that the rescaled FS $\left[\frac{\chi_F(t) - \chi_F(t_{\text{max}})}{\chi_F(t)}\right]$ is a simple function of the rescaled driving parameter $L'(t - t_{\text{max}})$. This function is universal and does not depend on system sizes, as shown in Fig. [4] for the case of $U = 30$, in which numerical results obtained from various system sizes fall onto a single line. On the other hand, if $t = t_{\text{max}}$ which approaches to $t_c$ like $t_{\text{max}} - t_c \propto L^{-2}$, the maximum value of the FS diverges with increasing system size as:

$$\chi_F(t = t_{\text{max}}) \propto L^{\mu}.$$  \hspace{1cm} (8)

which clearly differs from the Ising model. For the Ising model [Eq. (4)], 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 KT transition occurs at half-filling $n = 1$. The corresponding finite scaling analysis for the case $U = 30$ is presented in Fig. [4]. The maximum point of the FS is proportional to the system length. This is consistent with our aforementioned understanding. On the other hand, the rescaled FSs for various system sizes fall onto a single line, which is a function of $L'(t - t_{\text{max}})$ with critical length exponent $\nu = -1/4$. We find that the FS around the maximum point like:

$$\chi_F(t) \simeq 3.855 + 0.7478L + 1349.9L^{-1/2}(t - t_{\text{max}})^2.$$  \hspace{1cm} (9)

FIG. 2: (color online) The scaling behavior of the FS as a function of $t$ for the cases of $n = 1$ (LEFT) and $n = 2/3$ (RIGHT). Here $U = 10$.

FIG. 3: (color online) The finite size scaling is performed for the case of power-law divergence for the case of $U = 30$, $n = 2/3$, and system sizes $L = 6, 9, 12, 15$. The FS, consider as a function of the system size and the driving parameter is a function of $L'(t - t_{\text{max}})$ only. Here the critical exponent is $\nu \simeq 2.65$. The inset denotes the scaling behavior of $\chi_F(t = t_{\text{max}})$. The straight line is of slope 1 in logarithmic scale, and $\mu \simeq 5.3$.

FIG. 4: (color online) The similar finite size scaling is performed for the case of KT transition occurred for various system size $L = 6, 8, 10, 12$ at $n = 1$ and $U = 30$. The FS, consider as a function of the system size and the driving parameter is a function of $L'(t - t_{\text{max}})$ only. Here the critical exponent is $\nu \simeq -0.25$. The inset denotes the scaling behavior of $\chi_F(t = t_{\text{max}})$.
around $t_{\text{max}}$. As expected, there is no singularity in $\chi_{F(t)}(t)$. Clearly, the maximum behavior becomes weak with the increasing system size, as we can also find in Fig. 2. Then the FS becomes flat in the FK region, the relative larger FS is due to the power-law behavior the correlation function. On the other hand, motivated by the KT transition occurred in quantum XY model [23], we infer that the very steep decreasing point of the FS in Fig. 2 is more close to the critical point. Therefore, we perform $1/L$ finite scaling analysis for the minimum point of $d\chi_{F(t)}(t)/dt$, and find $t_c \simeq 0.308, 0.313, 0.317$ for $U = 10, 20, 30$ respectively. The results are very close to those obtained by density matrix renormalization group method [21].

A similar analysis can be carried on for other filling conditions. The power-law divergence of the FS always exists in other filling conditions except when $n = 1$. On the other hand, due to the particle-hole symmetry in the AHM, the FS takes the same value for $n$ and $2-n$ ($n < 2$), which satisfies the same scaling behavior. Therefore, the phase diagram in the left picture of Fig. 1 has a mirror symmetry about the line $n = 1$. Take into account the fact that even a single hole doping might lead to the instability of the density wave state in the infinite $U$ limit [27], the KT transition only happens at the half-filling condition. So the circle point in Fig. 1 is expected to be a quas-critical point in the phase diagram, and the FS just signals the transition type along the critical lines.

In conclusion, we have shown that the FS, as the leading term in the fidelity between two ground states separated by a slightly difference in 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 driving term in the Hamiltonian, the relation between the LSBT and FS is linked up. Its critical exponent then is naturally suitable for the classification of universality. We elucidate this relation by the simple QPT occurred in the 1D transverse-field Ising model. Furthermore, despite no singularity appearing in the FS when crossing a KT transition point, the stronger fluctuation might makes the FS reach a maximum near to the critical point. We then studied the FS in the 1D AHM, and shown that the FS can help us to identify both types of phase transition in this model. The critical exponent $\alpha$ for the Landau’s type transition is calculated with finite size analysis, and is found to be $\alpha = 2$ for $n = 2/3$ case. While for the KT transition, $\alpha = 0$.

Note added. Recently, the work on the scaling behavior of the FS in other model appeared [11].

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