Spectral function and fidelity susceptibility in quantum critical phenomena

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Abstract – In this paper, we derive a simple equality that relates the spectral function \( I(k, \omega) \) and the fidelity susceptibility \( \chi_F \), i.e. \( \chi_F = \lim_{\eta \to 0} \pi \eta I(0, i \eta) \) with \( \eta \) being the half-width of the resonance peak in the spectral function. Since the spectral function can be measured in experiments by the neutron scattering or the angle-resolved photoemission spectroscopy (ARPES) technique, our equality makes the fidelity susceptibility directly measurable in experiments. Physically, our equality reveals also that the resonance peak in the spectral function actually denotes a quantum criticality-like point at which the solid state seemly undergoes a significant change.

At zero temperature, the ground-state properties of a quantum many-body system can change quantitatively as the system’s parameter varies across a critical point. Because of the absence of thermal fluctuation, the quantitative change is solely driven by quantum fluctuation and hence it is called a quantum phase transition [1]. Examples of quantum phase transitions include Mott-insulator transitions and fractional quantum Hall liquids. In the recent decades, increasing attention has been paid to study quantum phase transitions from the perspectives of quantum information science [2], in particular using the concept of quantum entanglement [3,4] and quantum fidelity [5,6]. The application of these concepts does not require a prior knowledge of the symmetry of the system and makes them advantageous for the study. However, identifying an appropriate measure of the entanglement is highly non-trivial and there is still no unified theory on its role played in quantum phase transitions. A recent suggested proposal to detect the quantum critical points in experiments using bipartite fluctuations as a measure of the entanglement may provide an insight into this issue [7].

On the other hand, the fidelity approach to quantum phase transitions has a clearer physical picture. The ground-state wave functions on both sides of the critical point \( \lambda_c \) have distinct structures and if we compare two ground states separated by a small fixed distance \( \delta \lambda \) in the parameter space, i.e. the fidelity \( |\langle \psi_0(\lambda) | \psi_0(\lambda + \delta \lambda) \rangle| \), a minimum is expected to appear at the critical point \( \lambda_c \) [5,6]. The quantum phase transitions in the perspective of the fidelity have been verified in many strongly correlated systems [8–11]. Since the structure of the ground-state wave function undergoes a significant change as the system is driven adiabatically across the transition point, we can also imagine that the leading term of the fidelity, i.e. the fidelity susceptibility which denotes the leading response of the ground state to the driving parameter, should be a maximum or even divergent at the transition point [12,13]. Besides, the fidelity between two ground states separated by a long distance in the parameter space also manifests distinct information about quantum phase transitions [14,15]. Due to the remarkable properties of the fidelity around the critical point [15–18], the fidelity has become an efficient way to detect the quantum transition point in quantum many-body systems [19–30]. Especially, the fidelity has proven to be able to detect unconventional phase transitions such as the topological phase transition [20–23].

Despite the great success of the fidelity approach to quantum phase transitions in theory, little progress has been made in experiments. Up to now, the only experimental detection of the quantum phase transition in terms of fidelity is based on a spin dimer system via the technique of the nuclear-magnetic-resonance quantum simulator [31]. For a large quantum many-body system, say

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having a size $L > 10$, to measure the overlap of its two ground states separated by a short distance in the parameter space seems hard to be realized. The interesting scaling and universality behaviors of the fidelity susceptibility in quantum phase transitions still cannot be verified in experiments. Therefore, it is highly expected to find a way to measure the fidelity and its susceptibility directly or indirectly in experiments.

In this paper, we finally derive a neat equality that connects two seemingly unrelated quantities, i.e. the spectral function and fidelity susceptibility. Since the spectral function can be measured in experiments by, e.g., neutron scattering or the ARPES technique [32], such an equality actually makes the fidelity susceptibility directly measurable in experiments. On the other hand, as the most typical model in quantum phase transitions, the transverse-field Ising model and its quantum criticality now can be studied in experiment via neutron scattering [33]. A possible experimental scheme to measure the fidelity susceptibility of the transverse-field Ising model is proposed.

To begin with, we consider the propagation properties of a single electron in a solid-state system. Without loss of generality, we assume that the system can be described by a Hubbard-like model defined on a general lattice whose Hamiltonian reads

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

where $\langle \rangle$ denotes the summation over all the nearest-neighboring pairs, $c_{i \sigma}^\dagger$ ($c_{i \sigma}$) is the creation (annihilation) operator for electrons with spin $\sigma = \uparrow, \downarrow$ at site $i$, $t$ is the hoping integral, $n_{j \sigma} = c_{j \sigma}^\dagger c_{j \sigma}$, $U$ is the strength of the on-site Coulomb interaction. $H_V$ denotes other types of interactions such as coupling between the electrons in the system and the external applied magnetic field [34]. In a solid-state system, the total number of electrons is a good quantum number and is decided by the chemical potential of the system. Let us assume that the sample system has $N$ electrons. In this subspace, the eigenstates of the system are determined by the Schrödinger equation

$$H |\psi_n^N\rangle = E_n |\psi_n^N\rangle. \quad (2)$$

At zero temperature, the propagation of a single electron in the ground state $|\psi_0^N\rangle$ can be described by the one-electron Green’s function in the momentum-energy space,

$$G^\pm (k, \omega) = \sum_m \frac{|\langle \psi_m^N | \epsilon_k^\pm | \psi_0^N \rangle|^2}{\omega + E_m^N - E_{m+1}^N \pm i\eta}, \quad (3)$$

where $|\psi_m^N \rangle$ is the eigenstate of the Hamiltonian in the subspace of $N \pm 1$ electrons and $\epsilon_k^\pm = \epsilon_k^\uparrow - \epsilon_k^\downarrow$,

$$\epsilon_k^\pm = \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{k} \cdot \mathbf{r}_j} c_{j \sigma}^\mp \quad (4)$$

with $V$ being the volume of the system. Note that if one consider specifically the one-dimensional Hubbard model, the change in the ground-state wave function of the system could be obtained [35]. Nevertheless, we will leave our discussion general here. The one-electron spectral function

$$I^\pm (k, \omega) = -\frac{1}{\pi} \text{Im} G^\pm (k, \omega) \quad (5)$$

defines the one-electron addition and removal spectra. $I^\pm (k, \omega)$ can be probed in the inverse and direct photoemission, respectively [32]. From eq. (3), we have

$$I^\pm (k, \omega) = -\frac{1}{\pi} \sum_m \frac{|\langle \psi_m^N | \epsilon_k^\pm | \psi_0^N \rangle|^2}{\omega + E_m^N - E_{m+1}^N \pm \pi^2}. \quad (6)$$

We notice that the right-hand side of eq. (6) actually introduces the concept of dynamic fidelity susceptibility as defined in ref. [12]. To observe this, we need to consider the effective Hamiltonian including the subspace of both $N - 1$ and $N + 1$ electrons,

$$H(\eta) = \begin{pmatrix} H(N - 1) - \omega & \eta c_k^+ \\ \eta c_k & H(N) \end{pmatrix}, \quad (7)$$

where $\omega$ is due to the photon absorption and emission and $\eta$ is the strength of the perturbation. When $\eta = 0$, the initial ground state of the system $|\psi_0^N\rangle$ locates in the subspace of $N$ electrons. Then, if a small perturbation $\eta(c_k^+ + c_k)$ is turned on, the state becomes, to the first order,

$$|\psi_0(\eta)\rangle = |\psi_0^N\rangle + \eta \sum_m \frac{|\langle \psi_m^N | c_k^+ | \psi_0^N \rangle|^2}{\omega + E_m^N - E_{m+1}^N} |\psi_m^N\rangle$$

$$+ \eta \sum_m \frac{|\langle \psi_m^N | c_k^- | \psi_0^N \rangle|^2}{\omega + E_m^N - E_{m+1}^N} |\psi_m^N\rangle. \quad (8)$$

According to the definition [5], the fidelity between $|\psi_0^N\rangle$ and $|\psi_0(\eta)\rangle$ becomes

$$|\langle \psi_0^N | \psi_0(\eta) \rangle|^2 = 1 - \frac{\eta^2}{2} \chi_F + \cdots, \quad (9)$$

where

$$\chi_F = \sum_m \frac{|\langle \psi_m^N | c_k^+ | \psi_0^N \rangle|^2}{(\omega + E_m^N - E_{m+1}^N)^2}$$

$$+ \sum_m \frac{|\langle \psi_m^N | c_k^- | \psi_0^N \rangle|^2}{(\omega + E_m^N - E_{m+1}^N)^2} \quad (10)$$

is the so-called fidelity susceptibility. In ref. [12], we introduced the concept of dynamic fidelity susceptibility as

$$\chi_F(\eta) = \sum_m \frac{|\langle \psi_m^N | c_k^+ | \psi_0^N \rangle|^2}{(\omega + E_m^N - E_{m+1}^N)^2 + \eta^2}$$

$$+ \sum_m \frac{|\langle \psi_m^N | c_k^- | \psi_0^N \rangle|^2}{(\omega + E_m^N - E_{m+1}^N)^2 + \eta^2} \quad (11)$$
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Since \( I(\mathbf{k}, \omega) = I^+(\mathbf{k}, \omega) + I^-(\mathbf{k}, \omega) \), comparing the above equation with eq. (6), we obtain the following equality:

\[
I(\mathbf{k}, \omega) = \lim_{\eta \to 0} \frac{\eta}{\pi} \chi_F(\eta), \tag{12}
\]

or the inverse

\[
\chi_F = \lim_{\eta \to 0} \frac{\pi}{\eta} I(\mathbf{k}, \omega + i\eta), \tag{13}
\]

which is the key result of this work.

The equality about the fidelity susceptibility and the spectral function is remarkable. The former is a quantum information theoretic concept used to study quantum phase transitions. Physically, the divergence of the fidelity susceptibility manifests a significant change occurred in the structure of the ground-state wave function, hence denoting a phase transition. A lot of attention has been paid to the fidelity and fidelity susceptibility approach to quantum phase transitions in recent years [19]. Nevertheless, the corresponding experimental verification proved to be extremely difficult [31]. Equation (12) provides us a feasible way to measure the fidelity susceptibility in experiments via the neutron scattering or ARPES technique. Therefore, the equality makes the fidelity approach to quantum criticality not merely a theoretical topic. On the other hand, eq. (12) reveals that the resonance peak in the spectral function denotes a quantum criticality-like point at which the solid state of the sample system seemingly undergoes a significant change. Such an interpretation provides us a new angle to understand the spectral function from the viewpoint of quantum information science.

In ref. [12], when we defined the concept of dynamic fidelity susceptibility \( \chi_F(\eta) \), the variable \( \eta \) was introduced solely for a mathematical purpose to deal with the Fourier transformation in the complex plane. Since then, no work has ever touched the further meaning of \( \eta \). In the equality in eq. (12), we find it is \( \eta \) that connects the two seemingly unrelated quantities from two distinct fields. Moreover, \( \eta \) appends more physical understanding from the equality. From the definition of the fidelity susceptibility, \( \eta \) is the strength of the perturbation. While in the definition of the spectral function, \( \eta \) actually denotes the half-width of the resonance peaks. The uncertainty property of \( \eta \) even relates to the lifetime of the quasi-particle of the resonance peak.

To see the role of the equality in eq. (12) in quantum phase transitions, in the following, we take the one-dimensional transverse-field Ising model as an example to show how to measure the fidelity susceptibility in experiments. The model’s Hamiltonian reads

\[
H = -\sum_{j=1}^{N} \left( \sigma_j^x \sigma_{j+1}^x + h \sigma_j^z \right), \tag{14}
\]

where \( \sigma_j^{x,y,z} \) is the Pauli matrix for the 1/2 spin at site \( j \), \( h \) is the transverse field, and \( N \) is the number of spins. The periodic boundary conditions are assumed. The ground state of the Ising model has two distinct phases, which are the ferromagnetic phase favored by the ferromagnetic Ising interaction in the Hamiltonian and the paramagnetic phase due to the transverse field along +x-direction. The competition between them leads to a quantum phase transition occurring at \( h_c = 1 \).

The one-dimensional quantum Ising model can be realized by several materials. An excellent material is the insulating Ising ferromagnet CoNb$_2$O$_6$ whose spin dynamics can be measured by neutron scattering [33]. The model is defined on the zigzag structure formed by Co$^{2+}$ ions whose ferromagnetic coupling is about 1 meV (according to a magnetic field of 10 T $\sim$ 1 meV). Then the critical field of the systems is about \( h = 5.5 \) T which is attainable in the laboratory [33].

Theoretically, the model can be diagonalized by the Jordan-Wigner transformation

\[
\sigma_j^z = 1 - 2c_j^c c_j^\dagger, \quad \sigma_j^\dagger = \prod_{n<j} \sigma_n^x c_j^c c_j^\dagger, \tag{15}
\]

the Fourier transformation

\[
c_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k, \tag{16}
\]

and the Bogoliubov transformation

\[
c_k = u_k b_k + iv_k b_k^\dagger, \tag{17}
\]

where \( c_j \) is the annihilation operator for spinless fermions at site \( j \). With the diagonalization condition

\[
u_k^2 - v_k^2 = \cos 2\theta_k = \frac{-(\cos k - h)}{\sqrt{(\cos k - h)^2 + \sin^2 k}}, \tag{18}
\]

\[2uv_k \sin 2\theta_k = \frac{-\sin k}{\sqrt{(\cos k - h)^2 + \sin^2 k}}, \tag{19}\]

the Hamiltonian becomes

\[
H = \sum_k \epsilon(k) \left( 2b_k^\dagger b_k - 1 \right), \tag{20}
\]

where \( b_k \) and \( b_k^\dagger \) are fermionic operators, and \( \epsilon(k) = \sqrt{1 - 2h \cos(k) + h^2} \) is the dispersion relation of the quasi-particles of \( b_k^\dagger \).

Fidelity approach: From eq. (20), we see that the ground state of the system is the vacuum state of \( b_k^\dagger \), i.e. \( \langle 0 | b_k^\dagger \rangle = 0 \). Since \( b_k \) \( (b_k^\dagger) \) depends on the driving parameter \( h \), to compare the two ground states, we should define them in the space of \( c_k \) and \( c_k^\dagger \). The ground state can then be written as

\[
|\psi_0\rangle = \prod_{k>0} (\cos \theta_k |0_k, 0_{-k}) + e^{i\sin \theta_k} |1_k, 1_{-k})\rangle,
\]

where \( |1_k\rangle = c_k^\dagger |0_k\rangle \). Under the same basis, the fidelity between two ground states becomes

\[
F(h, h') = |\langle \psi_0(h) | \psi_0(h')\rangle| = \prod_{k>0} \cos(\theta_k - \theta_k').
\]
The fidelity susceptibility, as the leading term in the expansion of $F(h, h')$, can be calculated explicitly [5] as

$$\chi_F = \sum_{k > 0} \left( \frac{d\theta_k}{dh} \right)^2,$$

where

$$\frac{d\theta_k}{dh} = \frac{1}{2(1 - 2h \cos k + h^2)} \sin k.$$

The summation in eq. (21) can be carried out exactly and a closed form of the fidelity susceptibility in the model could be obtained [36].

**Spectral function:** In order to measure the fidelity susceptibility in experiments, we introduce

$$\sigma_k^\pm = \sum_i e^{\mp i\phi_i k} \sigma_i^\pm,$$

where $\sigma_j^+ + \sigma_j^- = \sigma_j^z$. Let $A_k = \sigma_k^+ + \sigma_k^-$, then $A_{k=0} = \sum_{j=1}^{N^z} \sigma_j^z$ is just the driving term of the Hamiltonian. The spectral function of $A_k$ can be written as

$$I(k, \omega + i\eta) = \sum_n \langle \psi_n | A_k | \psi_0 \rangle^2 \delta(E_0 - E_n + \omega + i\eta).$$

Let $k = 0$, $A_0 = N - 2 \sum_k \left[ (u_k^2 - v_k^2) b_k^\dagger b_k + iu_k v_k (b_k^\dagger b_{-k}^\dagger + b_k b_{-k}) + v_k^2 \right].$

Since the ground state is the vacuum state of $b_k$, the only contribution to the spectral function is the term $4 \sum_{k > 0} iu_k v_k b_k^\dagger b_{-k}^\dagger$. We find that the spectral function becomes

$$I(0, \omega + i\eta) = \sum_{k > 0} \frac{4 \sin^2 k}{\epsilon(k)^2} \delta[\epsilon(k) - \omega - i\eta].$$

In terms of the Poisson kernel representation of the $\delta$-function, we have

$$I(0, \omega + i\eta) = \sum_{k > 0} \frac{\eta}{\pi} \frac{4 \sin^2 k}{\epsilon(k)^2} \frac{1}{[\epsilon(k) - \omega]^2 + \eta^2}.$$
In summary, we derived an interesting equality that relates the fidelity susceptibility and spectral function. Such an equality makes it possible to measure the fidelity susceptibility directly in experiments via well-known techniques, such as neutron scattering, ARPES technique, etc. Then we investigated the feasibility of probing quantum criticality by measuring the fidelity susceptibility in experiments. For this purpose, we take the one-dimensional transverse-field Ising model as an example because the model can be realized by the compound material CoNb$_2$O$_6$ in the laboratory. We show that the fidelity susceptibility can be derived from the spectral function of the driving operator of the model. Due to the important role of the fidelity in detecting quantum phase transitions, we hope that the equality derived here will attract experimentalists to study critical phenomena by measuring the fidelity susceptibility directly in experiments.

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