Density-functional fidelity approach to quantum phase transitions

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We propose a new approach to quantum phase transitions in terms of the density-functional fidelity, which measures the similarity between density distributions of two ground states in parameter space. The key feature of the approach, as we will show, is that the density-functional fidelity can be measured easily in experiments. Both the validity and versatility of the approach are checked by the Lipkin-Meshkov-Glick model and the one-dimensional Hubbard model.

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**Motivation**—Recently, considerable attentions have been paid to the role of fidelity, a concept emerging from quantum information theory, in quantum phase transitions. Since the fidelity measures similarity of two quantum states without considering any order information in the states, its approach to quantum phase transitions has shed new lights on our understanding of the quantum criticality. For example, the fidelity and its leading term show singular and divergent behavior in the topological phase transition occurring in the ground states of both the Kitaev honeycomb model and the Kitaev toric model. While the topological phase transitions cannot be described by the Landau-Ginzburg-Wilson spontaneous symmetry-breaking theory. Mathematically, the fidelity is defined as an overlap between two ground states separated by a certain distance in the parameter space. To calculate the fidelity, one needs to know, in principle, all information of the ground states, including their each component in the Hilbert space of the Hamiltonian. This requirement is not an insurmountable barrier for theoretical studies because one can use some smart methods, for instance, the density-matrix-renormalization-group technique, to reduce the dimension of the Hilbert space. However, it might become a serious problem for experimental studies because to obtain the full ground-state function of a quantum many-body system is extremely difficult in experiments. This fact, to a certainty, obstructs experimentalists from measuring the ground-state fidelity of realistic quantum many-body systems.

Therefore, to find an appropriate approach that not only can describe the change in the ground-state structure in perspective of information theory, but also is based on experimentally measurable quantities, becomes a nontrivial problem. In this paper, we propose a new approach to quantum phase transitions in terms of the density-functional fidelity (DFF) and its susceptibility (DFFS). According to the Hohenberg-Kohn theorems, the ground-state properties of a quantum many-body system are uniquely determined by the density distribution \( n_x \) that minimizes the functional for the ground-state energy \( E_0[n_x] \). Therefore, the distribution \( n_x \) captures the most relevant information of the ground state. Any change in the structure of the wavefunction can be found by calculating the similarity between two density distributions, i.e., the DFF, directly. Since the density distribution is usually measurable in experiments, our approach, therefore, provides a practicable strategy to study quantum critical phenomena both theoretically and experimentally. To check both the validity and versatility of the approach, we take the Lipkin-Meshkov-Glick (LMG) model and the one-dimensional Hubbard model as examples, and study the DFF of real-space and momentum-space density distributions in the two models, respectively. We show that the real-space DFF is able to witness the second-order quantum phase transition occurring in the ground state of the LMG model in the anisotropic case; and the momentum-space DFF witness the Mott-insulator transition, which is of Beresinskii-Kosterlitz-Thouless (BKT) type, in the ground state of the Hubbard model.

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

\[
\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_I + \sum_x \mu_x \hat{n}_x, \tag{1}
\]

where \( \hat{H}_I \) is the interaction term and \( \lambda \) denotes strength, and \( \mu_x \) is the local (pseudo)potential associated with density distribution \( \{ n_x \} \). The index \( x \) can be discrete or continuous depending on the system under study. Though in the local-density-approximation (LDA) calculation, \( n_x \) usually refers to the density of electrons in real space, it can also be generalized to population in configuration space of a reduced-density matrix or the density of state in energy(momentum) space. The essence of the density-functional theory is that the density distribution has already capture the most relevant information of the ground state, any change in the environment conditions will leads another unique density distribution. In quantum information perspective, the density-functional theory can be used to calculate the ground-state entanglement in quantum many-body systems.

Mathematically, the single-particle state can be obtained by tracing out all other particles’ degree of free-
dom, i.e. \( \rho(x_1, x_1') = \text{tr}\{|\Psi_0(\lambda)\rangle\langle\Psi_0(\lambda)|\} \), where \( |\Psi_0(\lambda)\rangle \) is the ground state of the Hamiltonian \( \hat{H} \). Then the density distribution \( n \) is simply the diagonal part of the reduced-density matrix \( \rho(x_1, x_1') \)

\[
n = \sum_x n_x |x\rangle\langle x|, \quad n_x = \rho(x, x),
\]

where \( n \) has already been normalized. According to the Hellmann-Feynman theorem, the density distribution can also be obtained as

\[
n_x = \langle \Psi_0(\lambda)|\hat{n}_x|\Psi_0(\lambda)\rangle = \langle \Psi_0(\lambda)| (\partial \hat{H} / \partial \mu_x) |\Psi_0(\lambda)\rangle.
\]

Therefore, the change in the ground-state wavefunction can be reflected from the fidelity between the two density distributions. For two ground states at \( \lambda \) and \( \lambda' \), the DFF has the form,

\[
F(\lambda, \lambda') = \text{tr} \sqrt{n(\lambda)n(\lambda')}.
\]

If we fix the distance \( \delta\lambda = \lambda - \lambda' \), the DFF is expected to show a drop around the critical point because two ground states in different quantum phases has the maximum distance. In experiments, the density distribution \( n_x(\lambda) \) is measurable. Then the DFF between the density distributions under different environmental condition can be obtained.

Meanwhile, it was found that the fidelity susceptibility \( \chi_F \), which denotes the leading term of the fidelity, plays a central role in the fidelity approach to quantum phase transitions. Expanding the DFF to the leading order, we can find that

\[
F(\lambda, \lambda + \delta\lambda) = 1 - \frac{(\delta\lambda)^2}{2} \chi_F.
\]

where the DFFS \( \chi_F \) takes the form

\[
\chi_F = \sum_x \frac{1}{4n_x} \left( \frac{\partial n_x}{\partial \lambda} \right)^2.
\]

Therefore, if we regard \( \partial n_x / \partial \lambda \) as an independent function besides the density distribution \( n_x \), the DFF is a functional of \( n_x \) and \( \partial n_x / \partial \lambda \), both of which, in principle, maximize the DFFS at the critical point. The typical case might be that the density \( n_x \) in a certain region \( x_{\text{min}} < x < x_{\text{max}} \) vanishes (for \( 1/n_x \) rapidly) for \( \partial n_x / \partial \lambda \). These conclude the main formulism of the DFF approach to quantum phase transitions.

The Lipkin-Meshkov-Glick (LMG) model—To convince oneself of the validity of the approach, let us first study the DFF in a simple quantum phase transition occurring in the LMG model, which can provide us a clear paradigm of the approach. The Hamiltonian of the LMG model can be written as

\[
H = -\frac{\lambda}{2S} (1 + \gamma) \left( \hat{S}^2 - \hat{S}_z^2 - S \right) - 2\hbar \hat{S}_z - \frac{\lambda}{4S} (1 - \gamma) \left( \hat{S}_z^2 + \hat{S}_z^2 \right),
\]

where \( \hat{S}_a(a = x, y, z) \) is the spin-\( S \) operator and \( \hat{S}_z = \hat{S}_z + i\hat{S}_y \). The prefactor \( 1/S \) is necessary to ensure a finite \( E/S \) in the large \( S \) limit. It is understood that the total spin is the conserved quantities, i.e., \([\hat{H}, \hat{S}_a] = 0\). The ground state of the Hamiltonian locates in the subspace of maximum \( S \) and can be expressed in the basis of \( \hat{S}_z \), \( |\Psi_0(h)\rangle = \sum \varphi(s_z) |s_z\rangle \). Therefore, the ground-state energy is a density functional \( E_0[n_z] \), where \( n_z = \langle \Psi_0(h) | \hat{s}_z | \Psi_0(h) \rangle \) with \( \hat{s}_z = |s_z\rangle \langle s_z| \).

The ground state of the LMG model in the anisotropic case \( (\gamma \neq 1) \) consists of two phases, i.e the polarized phase for \( h > 1 \), and the symmetry-breaking phase for \( 0 < h < 1 \). A simple quantum phase transition occurs at the critical point \( h_c = 1 \). For an illustrative purpose, we show the density distributions \( n_z \) as a function of \( s_z \) for a sample of \( S = 2048 \) under various \( h \) is in Fig. 1 (a). When \( h < 1 \), the density distribution \( n_z \) always shows a peak which is dragged to the boundary of maximum \( s_z \) little by little as \( h \) increases. The DFF can be sketched out from the overlap between two neighboring distributions, which becomes smaller and smaller, and finally reaches a minimum around \( h_c = 1 \). When \( h > 1 \), the density peak diverges. In this case, a small change of \( h \) can not change the density distribution significantly, then the DFF is close to 1 again. Fig. 1 (b) represents the DFF as a function of \( h \) for \( \delta h = 0.005 \). Clearly the sudden drop of the DFF corresponds the second-order quantum phase transition. The sharp peak in the DFF susceptibility [Fig. 1 (c)] implies that the density distribution evolves dramatically around the critical point.

For the LMG model, \( n_z = \varphi(s_z) \varphi(s_z) \), so the DFF is mathematically the same as the previously studied ground-state fidelity \( \chi^2 \), hence satisfies the same scaling and critical behaviors as the ground-state fidelity.
However, we would like to emphasize here that the motivation of the DFF is quite different. The mathematical coincidence of two fidelities of the LMG model is due to the fact that the model in the subspace of maximum $S$ becomes a single-particle problem. In this case, the diagonal element of the single-particle reduced-density matrix is just the absolute value of the wavefunction.

The one-dimensional Hubbard model—The density distribution in the density-functional theory can be generalized to any density distribution, for instance, the density of state. To see the versatility of the approach, here we take the one-dimensional Hubbard model [32, 35] to show how the change in the density of state in momentum space around the critical point can be reflected from the corresponding DFF and DFFS. The Hamiltonian of the one-dimensional Hubbard model reads

$$H = - \sum_{\sigma,j=1}^{L} (\hat{c}_{j+1,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma}) + U \sum_{j} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow},$$

where $\hat{c}_{j,\sigma}^\dagger$ and $\hat{c}_{j,\sigma}$ are creation and annihilation operators for fermionic atoms with spin $\sigma$ at site $j$, respectively. $\hat{n}_{j,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma}$, and $U$ denotes the strength of on-site interaction. The Hubbard model can be solved exactly via the Bethe-ansatz method [35]. For the case of $U > 0$ and $N \leq L$, the energy spectra of the system under the periodic boundary conditions are determined by a set of charge and spin rapidities $\{k_j, \lambda_n\}$, which satisfy the following transcendental Bethe-ansatz equations (BAEs)

$$2\pi I_j = k_j L - \sum_{a=1}^{M} \theta_1(\lambda_a - \sin k_j),$$

$$2\pi J_a = \sum_{j=1}^{N} \theta_1(\lambda_a - \sin k_j) - \sum_{b=1}^{M} \theta_2(\lambda_a - \lambda_b),$$

where $\theta_1(x) = 2 \tan^{-1} (4k/nU)$, $M$ is the number of down spins and $\{I_j, J_a\}$ play the role of quantum number. The ground-state solution only consists of real $k$s and real $\lambda$s. It is a singlet state, given by a quantum number configuration (successive integers or half-odd-integers) symmetrically arranged around zero. Once the rapidities $\{k_j, \lambda_n\}$ are obtained from Eqs. (9, 10), the energy of the state can be calculated as $E = -2 \sum_j \cos k_j$.

For the half-filled case, i.e $N = L$, a Mott-insulator transition occurs at the critical point $U = 0$. If $U > 0$, a charge gap opens and the system becomes an insulator. The ground-state energy the Hubbard model around $U = 0$ is infinitely differentiable, the phase transition belongs to the BKT type. Recent entanglement approach to the Hubbard model [33, 34] shows that single-site entanglement shows a maximum, due to the various correlations have long-range behaviors, at the critical point. However, whether the ground-state fidelity can witness the Mott-insulator transition is still controversial [18]. To apply the DFF approach to the phase transition, we use the concept of the density of state in the quasi-momentum space that is defined as $\rho'(k_{j+1} + k_j)/2 = 1/[L(k_{j+1} + k_j)]$. Then the ground-state energy can be calculated as $E = -(N/\pi) \int_{-\pi}^{\pi} dk \rho(k) \cos k$. Clearly, the density of state $\rho(k)$ uniquely decides the ground-state energy.

To see the evolution in the density of state, in Fig. 2, (a) we show the density of state for a system of $L = N = 210$ and a set of uniformly distributed $U$ with space $\delta U = 0.04$. From the figure, we can see that if $U$ is large, the densities of state are very close, this observation means that the DFF between two closing densities is almost 1 [See Fig. 2 (b)]. The underlying physical picture is that, in the large $U$ limit, the system becomes a full-filled spinless fermion model, the $k$s in Eq. (9) are almost uniformly distributed, then the density of state is very flat in the momentum space. On the other hand, as $U$ becomes smaller and smaller, the second term of Eq. (9) makes any $k$ more close to the zero point hence suppresses the density of state in the region of $|k| > \pi/2$, while increase $\rho(k)$ in $|k| < \pi/2$. The physics is straightforward. The Pauli’s exclusion principle does not forbidden two electrons with different spin polarizations to occupy the same state in $k$ space. To have a low energy, electrons want to stay as close as possible to the $k = 0$ point. Then the density of state become higher in $|k| < \pi/2$ and smaller in $|k| > \pi/2$ as $U$ decreases. Around the critical point, the change in the density of state becomes dramatic. Then the DFF deviates from 1 little by little, and the fidelity susceptibility becomes larger and larger. Though the Bethe-ansatz equations are extremely difficult to be solved around $U = 0$, we can still find the DFFS tends to a maximum as $U$ tends to zero.

We can also check the above picture analytically in some special cases. In the thermodynamic limit and half-
filled case, the density of state is
\[
\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi} \int_0^{\infty} dp J_0(p) \cos(p \sin k) \frac{e^{-|p|}}{1 + e^{U/|p|/8}},
\]
(11)
where \(J_0\) is zeroth order Bessel function. If \(U = \infty\), the second term of Eq. (11) vanishes, so \(\rho(k) = 1/(2\pi)\) for \(k \in [-\pi, \pi]\). If \(U = 0\), since \(\int_0^{\infty} dp J_0(p) \cos(p \sin k) = |\cos k|^{-1}\), so \(\rho(k) = 1/\pi\) for \(k \in [-\pi/2, \pi/2]\) and \(\rho(k) = 0\) for \(|k| > \pi/2\). This tells us that the density of state undergoes a dramatic change around the critical point. Therefore, as implied from the Eq. (10), the DFF should reaches a maximum at the critical point \(U = 0\).

In summary, we have proposed a new approach to quantum phase transitions based on the DFF and DFFS. The former measures the similarity between two density distributions and the latter describes the changing rate of the density distribution in the parameter space. We show that the divergence of the DFFS is typically related to a quickly vanishing density distribution, which actually denotes a quantum phase transition. To check the validity of the approach, we studied the DFF in the LMG model and show that the divergence of the DFF at the critical point. Also to see the versatility of the approach, we studied the DFF for the density of state of the one-dimensional Hubbard model. As the on-site \(U\) tends to zero, the density of state in the regions \([-\pi,-\pi/2]\) and \([\pi/2, \pi]\) quickly vanishes. This phenomena leads a maximized (at least) DFFS around the critical point \(U = 0\).

Though we restricted out studies in two well-studied strongly correlated systems, the approach we proposed can be applied to any quantum systems. Especially, the DFF approach can be used to study various quantum phase transitions (like the structural phase transition) based the LDA calculations.

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