Bifurcation in ground-state fidelity and universal order parameter for two-dimensional quantum transverse Ising model

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We establish an intriguing connection between quantum phase transitions and bifurcations in the ground-state fidelity per lattice site, and construct the universal order parameter for quantum Ising model in a transverse magnetic field on an infinite-size square lattice in two spatial dimensions, a prototypical model with symmetry breaking order. This is achieved by computing ground-state wave functions in the context of the tensor network algorithm based on the infinite projected entangled-pair state representation. Our finding is applicable to any systems with symmetry breaking order, as a result of the fact that, in the conventional Landau-Ginzburg-Wilson paradigm, a quantum system undergoing a phase transition is characterized in terms of spontaneous symmetry breaking captured by a local order parameter. In addition, a bifurcation in the reduced fidelity between two different reduced density matrices is also discussed.

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I. INTRODUCTION

In recent years, a novel approach to quantum phase transitions (PQ Ts) [1, 2] in quantum many-body lattice systems emerges, based on the fact that fidelity, a basic notion in quantum information science, is a measure of quantum state distinguishability [3–12]. As argued in Refs. [4–9], the ground-state fidelity per lattice site captures drastic changes of the ground-state wave functions around a critical point for a quantum system in any spatial dimensions. That is, it is a universal marker to detect QPTs, regardless of what type of the internal order is present. In fact, quantum many-body lattice systems with either spontaneous symmetry breaking (SSB) order or topological order, have been specifically studied: for the former, the examples include quantum transverse Ising [8] and Potts chains [13], quantum Ising [7] and XYX models [14] on a square lattice, while for the latter, the Kitaev model [15] on a honeycomb lattice. Remarkably, there is a smoking-gun signature for SSB order in the fidelity per site approach: SSB order implies a bifurcation, arising from degenerate ground-state wave functions due to broken symmetry, in the ground-state fidelity per lattice site.

In fact, it was shown that, for a QPT arising from an SSB, a bifurcation appears in the ground-state fidelity per site, with a critical point identified as a bifurcation point. This in turn results in a novel concept of the universal order parameter, which appears as the ground-state fidelity per lattice site between a ground state and its symmetry-transformed counterpart. The advantage of the ground-state fidelity per lattice site and the universal order parameter [16] over local order parameters lies in the fact that both of them are universal, in the sense that it is not model-dependent, in contrast to model-dependent order parameters in characterizing QPTs in quantum lattice many-body systems. Similarly, a bifurcation occurs in the ground-state reduced fidelity [17] between the one-site reduced density matrices and the two-site reduced density matrices, with a critical point identified as a bifurcation point. However, all specific examples, up to now, have been restricted to quantum many-body lattice systems in one spatial dimension.

In this paper, we take one step further to see if these novel ideas are practical to quantum many-body lattice systems in two spatial dimensions. We establish, by exploiting the tensor network algorithm based on the infinite projected entangled-pair states (iPEPS) algorithm [18], an intriguing connection between a QPT and a bifurcation in the ground-state fidelity per lattice site, and construct the universal order parameter for quantum transverse Ising model on a square lattice, a prototypical model with symmetry breaking order. Our finding is applicable to any systems with symmetry breaking order, as a result of the fact that, in the conventional Landau-Ginzburg-Wilson paradigm, a quantum system undergoing a phase transition is characterized in terms of SSB captured by a local order parameter. In addition, a bifurcation in the reduced fidelity between two different reduced density matrices is also discussed.

II. MODEL

We consider quantum Ising model in a transverse magnetic field on an infinite-size square lattice in two spatial dimensions. It is described by the Hamiltonian:

\[ H = -\sum_{\langle ij \rangle} \sigma^x_i \sigma^x_j + \lambda \sum_i \sigma^z_i, \]

where \( \sigma^\alpha_i \) (\( \alpha = x, z \)) are the spin 1/2 Pauli operators at site \( i \), \( \langle ij \rangle \) runs over all the possible nearest-neighbor pairs on a square lattice, and \( \lambda \) is the transverse magnetic field, which we choose as a control parameter. The model is invariant under the symmetry operation: \( \sigma^x_i \to -\sigma^x_i \) and \( \sigma^z_i \to \sigma^z_i \) for all sites simultaneously, which yields the \( \mathbb{Z}_2 \) symmetry. As is well known, the system undergoes a second-order QPTs at the critical field \( \lambda_c \sim 3.044 \) [18, 19].
III. BIFURCATION IN THE GROUND-STATE FIDELITY PER LATTICE SITE

For two ground-state wave functions $|\Psi(\lambda_1)\rangle$ and $|\Psi(\lambda_2)\rangle$ corresponding to two different values $\lambda_1$ and $\lambda_2$ of the control parameter $\lambda$, the ground-state fidelity $F(\lambda_1, \lambda_2) = \langle \Psi(\lambda_2) | \Psi(\lambda_1) \rangle$ asymptotically scales as $F(\lambda_1, \lambda_2) \sim d(\lambda_1, \lambda_2)^{N/4}$, with $N$ being the number of sites in the lattice. Here, $d(\lambda_1, \lambda_2)$ is the scaling parameter, introduced for one-dimensional quantum systems [4–6] and for two and higher-dimensional quantum systems [7]. Note that it characterizes how fast fidelity goes to zero when the thermodynamic limit is approached. Physically, the scaling parameter $d(\lambda_1, \lambda_2)$ is the averaged fidelity per lattice site, which is well defined in the thermodynamic limit:

$$\ln d(\lambda_1, \lambda_2) \equiv \lim_{N \to \infty} \ln \frac{F(\lambda_1, \lambda_2)}{N}. \quad (2)$$

As noted in Refs. [4–6, 7], it satisfies the properties inherited from the fidelity $F(\lambda_1, \lambda_2)$: (i) normalization $d(\lambda, \lambda) = 1$; (ii) symmetry $d(\lambda_1, \lambda_2) = d(\lambda_2, \lambda_1)$; and (iii) range $0 \leq d(\lambda_1, \lambda_2) \leq 1$.

In the $Z_2$ symmetric phase, the ground-state wave function is non-degenerate, while in the $Z_2$ symmetry-broken phase, two degenerate ground-state wave functions arise. If we choose $|\Psi(\lambda_2)\rangle$ as a reference state, with $\lambda_2$ in the $Z_2$ symmetric phase, then the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, is not able to distinguish two degenerate ground-state wave functions in the $Z_2$ symmetry-broken phase. However, if we choose $|\Psi(\lambda_2)\rangle$ as a reference state, with $\lambda_2$ in the $Z_2$ symmetry-broken phase, then the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, can be used to distinguish two degenerate ground-state wave functions. Therefore, a bifurcation occurs in the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, as a function of $\lambda_1$, for a fixed $\lambda_2$. As argued in Refs. [8, 9], for a given truncation dimension $D$, a pseudo-phase-transition point $\lambda_D$ manifests itself as a bifurcation point [20].

In Fig. 1 we plot the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, for quantum Ising model in a transverse magnetic field on an infinite-size square lattice in two spatial dimensions, with the transverse magnetic field $\lambda$ as the control parameter. Note that a bifurcation does occur for the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$. Here, we have chosen $\lambda_2 = 2.1$ as a specific example. The pseudo-phase-transition point locates at $\lambda_D = 3.100$ for the truncation dimension $D = 2$, at $\lambda_D = 3.065$ for the truncation dimension $D = 3$, and at $\lambda_D = 3.050$ for the truncation dimension $D = 4$. We mention that the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, is computed from the iPEPS representation of the ground-state wave functions, following the transfer matrix approach described in Ref. [7].

A remarkable feature of the bifurcation points for the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, as seen in Fig. 1 is that $d(\lambda_1, \lambda_2)$ between different symmetry breaking ground-state wave functions in the same phase appears less than that between two ground-state wave functions from different phases. This is due to the fact that two degenerate symmetry breaking ground states in the same symmetry-broken phase are more distinguishable than two ground states from different phases.

IV. THE GROUND-STATE REDUCED FIDELITY BETWEEN TWO REDUCED DENSITY MATRICES

For quantum Ising model in a transverse magnetic field on an infinite-size square lattice, the one-site reduced density matrix in the $Z_2$ symmetric phase takes the form,

$$\rho = \frac{1}{2} + 2 \langle S_z \rangle S_z, \quad (3)$$

where $\langle S_z \rangle$ is the ground-state expectation value of $S_z$ in the $Z_2$ symmetric phase, while the two-site reduced density matrix is,

$$\rho = \frac{1}{4} I + 4 \gamma_{xx} S_x \otimes S_x + 4 \gamma_{yz} S_z \otimes S_z + \gamma_{xz} I \otimes S_z + \gamma_{zy} S_z \otimes I. \quad (4)$$

Here, $\gamma_{xx} = \langle S_x \otimes S_x \rangle$, $\gamma_{zz} = \langle S_z \otimes S_z \rangle$, $\gamma_{zy} = \langle I \otimes S_z \rangle$, $\gamma_{xz} = \langle S_z \otimes I \rangle$, and $I$ is the identity matrix.

In the $Z_2$ symmetry-broken phase, the one-site reduced density matrix becomes,

$$\rho = \frac{1}{2} + 2 \langle S_x \rangle S_x + 2 \langle S_z \rangle S_z, \quad (5)$$

whereas the two-site reduced density matrix is

$$\rho = \frac{1}{4} I + 4 \gamma_{xx} S_x \otimes S_x + 4 \gamma_{yz} S_z \otimes S_z + \gamma_{xz} I \otimes S_z + \gamma_{zy} S_z \otimes I + 4 \gamma_{xz} S_z \otimes S_z + \gamma_{oz} I \otimes S_x + \gamma_{ox} S_x \otimes I, \quad (6)$$

FIG. 1: (color online) The ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, for quantum Ising model in a transverse field on a square lattice in two spatial dimensions, with the transverse magnetic field $\lambda$ as the control parameter. If we choose $|\Psi(\lambda_2)\rangle$ as a reference state, with $\lambda_2$ being in the $Z_2$ symmetry-broken phase, then $d(\lambda_1, \lambda_2)$ distinguishes two degenerate ground-state wave functions, with a pseudo-phase-transition point $\lambda_D$ as a bifurcation point. Here, we have chosen $\lambda_2 = 2.1$. The pseudo-phase-transition point is identified at $\lambda_D = 3.100$ for the truncation dimension $D = 2$, at $\lambda_D = 3.065$ for the truncation dimension $D = 3$, and at $\lambda_D = 3.050$ for the truncation dimension $D = 4$, respectively.
with $\gamma_{xx} = \langle S_x \otimes S_x \rangle$, $\gamma_{zz} = \langle S_z \otimes S_z \rangle$, $\gamma_{xx} = \langle I \otimes S_x \rangle$, and $\gamma_{zz} = \langle S_z \otimes I \rangle$.

The reduced fidelity measures the distance between two quantum mixed states. For two reduced density matrices $\rho_{1\lambda}$ and $\rho_{1\lambda}$, the reduced fidelity $F(\rho_{1\lambda}, \rho_{2\lambda})$ is defined to be [17]

$$F(\rho_{1\lambda}, \rho_{2\lambda}) = \text{tr} \sqrt{\rho_{1\lambda}^{1/2} \rho_{2\lambda}^{1/2}}. \quad (7)$$

Here, $\rho_{1\lambda}$ and $\rho_{2\lambda}$ are the reduced density matrices corresponding to two different values, $\lambda_1$ and $\lambda_2$, of the control parameter $\lambda$. Notice that the reduced fidelity $F(\rho_{1\lambda}, \rho_{2\lambda})$ is a function of $\lambda_1$ and $\lambda_2$, which satisfies the following properties: (i) normalization $F(\rho_{1\lambda}, \rho_{1\lambda}) = 1$; (ii) symmetry $F(\rho_{1\lambda}, \rho_{2\lambda}) = F(\rho_{2\lambda}, \rho_{1\lambda})$; (iii) range $0 \leq F(\rho_{1\lambda}, \rho_{2\lambda}) \leq 1$.

In Fig. 2 (upper panel), we plot the ground-state reduced fidelity $F(\rho_{1\lambda}, \rho_{1\lambda})$ between the one-site reduced density matrices for quantum Ising model in a transverse field on an infinite-size square lattice, with the transverse field strength $\lambda$ as the control parameter. Here, we choose $\rho_{1\lambda}$, at $\lambda_2 = 2.1$, as a reference state, which breaks the $Z_2$ symmetry. The one-site reduced fidelity is able to distinguish two mixed states (described by two reduced density matrices) from two degenerate ground-state wave functions, with a bifurcation point as a pseudo-phase-transition point $\lambda_{\text{B}}$. When the control parameter $\lambda$ crosses a pseudo-transition point, the ground-state degeneracy changes suddenly, implying that the system undergoes a QPT. We observe that the pseudo-phase-transition point $\lambda_{\text{B}}$ moves toward the critical point $\lambda_c$ with increasing $D$.

More precisely, the pseudo-phase-transition point locates at $\lambda_{\text{B}} = 3.100$ for the truncation dimension $D = 2$, at $\lambda_{\text{B}} = 3.065$ for the truncation dimension $D = 3$, and at $\lambda_{\text{B}} = 3.050$ for the truncation dimension $D = 4$, respectively.

We also plot the ground-state reduced fidelity $F(\rho_{1\lambda}, \rho_{2\lambda})$ between the two-site reduced density matrices for quantum Ising model in a transverse field on an infinite-size square lattice in Fig. 2 (lower panel). The reference state is chosen at the same $\lambda_2 = 2.1$, as in the case of the one-site reduced fidelity. We observe that a bifurcation also occurs in the two-site reduced fidelity, with the same pseudo-phase-transition point $\lambda_{\text{B}}$. This is expected, simply because they are resulted from the same set of the ground-state wave functions.

V. THE UNIVERSAL ORDER PARAMETER

As argued in Ref. [16], for any quantum lattice system with a symmetry group $G$ undergoing a QPT with symmetry breaking order, there is a universal order parameter: it is defined as the ground state fidelity per lattice site between a ground-state wave function and its symmetry-transformed counterpart, which is discontinuous for first-order phase transitions and continuous for second-order phase transitions. This is based on the observation that, for any ground state $|\Psi\rangle$ in the symmetric phase, $\langle \Psi_g | \Psi \rangle$ is equal to 1, for any symmetry operation $g \in G$, whereas it is identical to zero for any state in the symmetry broken phase.

In order to measure the distance between two quantum states $|\Psi(\lambda)\rangle$ and $g|\Psi(\lambda)\rangle$, let us consider their counterparts $|\Psi_g(\lambda)\rangle$ and $g|\Psi_g(\lambda)\rangle$ on a finite-size lattice, with $L$ being the number of the total lattice sites. As argued in Refs. [4–7], $L|\langle \Psi | \Psi \rangle|_L$ asymptotically scales as $f^L_\lambda(\lambda)$ with $L$, as one may see from the tensor network representations of the system’s ground state wave functions. Here, $f^L_\lambda(\lambda)$ is the averaged fidelity per lattice site, which is well-defined even in the thermodynamic limit. As such, one sees that, $f^L_\lambda(\lambda) = 1$ for any $g \in G$, if $\lambda$ is in the symmetric phase $\lambda > \lambda_c$, and $0 < f^L_\lambda(\lambda) < 1$ for any nontrivial symmetry operation $g$, if $\lambda$ is in the symmetry-broken phase $\lambda < \lambda_c$. As argued in Ref. [16], we define the universal order parameter to be

$$I_\lambda = \sqrt{1 - f^L_\lambda(\lambda)}. \quad (8)$$

Note that $I_\lambda(\lambda)$ is always zero if $\lambda > \lambda_c$. However, it becomes nonzero, with its value ranging from 0 to 1, if $\lambda < \lambda_c$. These features are exactly what one requires for $I_\lambda(\lambda)$ to be an order parameter. In fact, this is valid for any quantum many-body lattice system with a global symmetry group $G$ spontaneously broken. A remarkable feature of the universal order parameter
FIG. 3: (color online) The universal order parameter $I(\lambda)$ for quantum Ising model in a transverse magnetic field on a square lattice. A pseudo-phase-transition point $\lambda_D$ occurs, as $I(\lambda)$ changes from being nonzero to zero at $\lambda = \lambda_D$. When the truncation dimension $D$ is increased, a pseudo-phase-transition point $\lambda_D$ approaches the critical point $\lambda_c$. In addition, the universal order parameter $I(\lambda)$ reaches the maximum value $I(\lambda) = 1$ at the factorizing field $\lambda_f = 0$.

is that it not only makes it possible to locate a critical point, but also enables us to identify a factorized state $\ket{\Psi(\lambda_f)}$, with $\lambda_f$ being the so-called factorizing field [21].

In Fig.3, we plot the universal order parameter $I_g(\lambda)$ for quantum Ising model in a transverse field on an infinite-size square lattice, with the field strength $\lambda$ as the control parameter. Here, the symmetry operation is the non-trivial element $g$ of the group $Z_2$. If $\lambda < \lambda_D$, the universal order parameter $I_g(\lambda)$ is non-zero. This characterizes the $Z_2$ symmetry-broken phase, in contrast to the fact that the universal order parameter $I_g(\lambda)$ is zero, in the symmetric phase $\lambda > \lambda_D$. As the control parameter $\lambda$ varies across the pseudo-critical point $\lambda_D$, the behavior of the universal order parameter $I_g(\lambda)$ changes qualitatively, implying that the system undergoes a QPT at the pseudo-phase-transition point $\lambda_D$. As the truncation dimension $D$ is increased, the pseudo-phase-transition point $\lambda_D$ moves toward the critical point $\lambda_c$. In addition, the (trivial) factorizing field $\lambda_f = 0$ exists for quantum Ising model in a transverse field on an infinite-size square lattice, at which $I_g(\lambda)$ reaches its maximum.

VI. CONCLUSIONS
We have investigated an intriguing connection between QPTs and bifurcations in the ground-state fidelity per lattice site, in the context of the tensor network algorithm based on the iPEPS representation. For quantum transverse Ising model on an infinite-size square lattice, the iPEPS algorithm produces two degenerate symmetry-breaking ground-state wave functions arising from the $Z_2$ symmetry breaking, each of which results from a randomly chosen initial state. Therefore, a quantum system undergoing a phase transition is characterized in terms of SSB that is captured by a bifurcation in the ground-state fidelity per lattice site. We have also constructed the universal order parameter, and discussed bifurcations in the ground-state reduced fidelity between two different reduced density matrices in the symmetry-broken phase, for quantum Ising model in a transverse magnetic field on an infinite-size square lattice. We expect that our approach might provide further insights into critical phenomena in quantum many-body lattice systems in condensed matter.

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