Ground State Fidelity from Tensor Network Representations

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For any D-dimensional quantum lattice system, the fidelity between two ground state many-body wave functions is mapped onto the partition function of a D-dimensional classical statistical vertex lattice model with the same lattice geometry. The fidelity per lattice site, analogous to the free energy per site, is well defined in the thermodynamic limit and can be used to characterize the phase diagram of the model. We explain how to compute the fidelity per site in the context of tensor network algorithms, and demonstrate the approach by analyzing the two-dimensional quantum Ising model with transverse and parallel magnetic fields.

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The discoveries of high-T_c superconductors and fractional quantum Hall liquids have stimulated a surge of activities in the study of quantum phase transitions (QPTs) [1]. The conventional description of QPTs in condensed matter physics is in terms of orders and fluctuations. The Landau-Ginzburg-Wilson paradigm describes symmetry-breaking orders quantified by a local order parameter, whose nonzero value characterizes a symmetry-broken phase. Continuous QPTs beyond the Landau-Ginzburg-Wilson paradigm also exist. They are described in terms of the so-called topological or quantum orders [2] and are relevant to emergent phenomena in strongly correlated electron systems, with nonlocal order parameters as a salient feature.

By using concepts of quantum information science, recently two new approaches to study QPTs have been proposed. They focus on properties of ground state wave functions of the quantum many-body system, namely *entanglement* [3–9] and *fidelity* [10–12], and turn out to be very successful at detecting quantum critical behaviors. In particular, the entanglement entropy is exploited to reveal qualitatively different behaviors at and off quantum criticality [5,6], whereas the fidelity, a measure of distinguishability of states in the system's Hilbert space, is shown to be able to capture drastic changes in quantum ground states when the system undergoes a QPT, regardless of what type of internal order is present [11]. Both approaches have been shown to be insightful in the context of already well-understood systems, but in practice, when applied to a generic system, they still rely on our ability to compute certain properties of ground state wave functions, which is in general a very difficult task.

On the other hand, significant progress has also been made recently in the classical simulation of quantum many-body systems by using a *tensor network* (TN) to represent the wave function. Examples of TNs include a matrix product state (MPS) [13–15] for systems in one spatial dimension and the projected entangled-pair state (PEPS) [16] in two and higher spatial dimensions. For systems invariant under translations, particularly efficient algorithms have been proposed to compute the ground state for infinite systems, both in one [17] and two [18] spatial dimensions, as well as for finite systems with periodic boundary conditions (PBC) [19].

The purpose of this Letter is twofold. We consider a system, either infinite or finite with PBC, defined on a D-dimensional lattice and such that its ground state is invariant under translations [20]. First, we show that the fidelity between two ground states can be mapped onto the partition function of a D-dimensional classical statistical vertex lattice model with the same lattice geometry. This is achieved by exploiting the fact that the two ground states can be represented in terms of a TN where all the tensors are copies of one single tensor. The fidelity per lattice site, introduced in Ref. [11], is naturally interpreted as the free energy per site of this D-dimensional classical statistical vertex lattice model, and as such it is well defined in the thermodynamic limit (even though the fidelity itself becomes zero). Second, we consider the practical computation of the fidelity per lattice site, both for finite and infinite systems, within the framework of TN algorithms for translationally invariant systems [17–19]. As a result, we obtain a viable scheme to determine the ground state phase diagram of a system without prior knowledge of order parameters. We demonstrate the approach by analyzing the two-dimensional quantum Ising model with both transverse and parallel magnetic fields. First and second order phase transitions, as well as stable fixed points, are clearly identified.

Generalities.—Consider a finite quantum lattice system S in D dimensions described by a Hamiltonian $H(\lambda)$, where λ is a control parameter [21]. For two ground states $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ corresponding to two different values λ_1 and λ_2 of the control parameter λ, the ground state fidelity $F(\lambda_1, \lambda_2) = |\langle\psi(\lambda_2)|\psi(\lambda_1)\rangle|$ asymptotically scales as $F(\lambda_1, \lambda_2) \sim d(\lambda_1, \lambda_2)^N$, with N the number of sites in the lattice. Here, $d(\lambda_1, \lambda_2)$ is the scaling parameter, introduced in Ref. [11] for one-dimensional quantum systems,

which characterizes how fast the 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,

$$\ln d(\lambda_1, \lambda_2) \equiv \lim_{N\to\infty} \frac{\ln F(\lambda_1, \lambda_2)}{N}, \tag{1}$$

which is seen to be well defined in the thermodynamic limit even if $F(\lambda_1, \lambda_2)$ becomes trivially zero. 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 $0 \le d(\lambda_1, \lambda_2) \le 1$. Additionally, in a finite system, we can define a finite-size analogue of $d(\lambda_1, \lambda_2)$ through

$$\ln d_N(\lambda_1, \lambda_2) \equiv \frac{\ln F(\lambda_1, \lambda_2)}{N}. \tag{2}$$

As argued in Ref. [11], the fidelity per lattice site $d(\lambda_1, \lambda_2)$ succeeds in capturing nontrivial information including stable and unstable fixed points along renormalization group flows. Specifically, suppose the system S undergoes a QPT at a transition point λ_c. Then, $d(\lambda_1, \lambda_2)$ exhibits singular behaviors when λ_1 crosses λ_c for a fixed λ_2, or λ_2 crosses λ_c for a fixed λ_1. That is, a transition point λ_c is characterized as a *pinch point* (λ_c, λ_c) for *continuous* QPTs: the intersection of two singular lines $\lambda_1 = \lambda_c$ and $\lambda_2 = \lambda_c$ on the two-dimensional surface defined by $d(\lambda_1, \lambda_2)$ as a function of λ_1 and λ_2. For first order QPTs, $d(\lambda_1, \lambda_2)$ becomes discontinuous (as either λ_1 or λ_2 crosses a transition point) [22].

Mapping onto a D-dimensional classical statistical vertex lattice model.— As it is well known, there is a remarkable mapping from a D-dimensional quantum system to an equivalent $(D + 1)$-dimensional classical system with imaginary time as an extra dimension [23,24]. Here, we discuss another mapping, one from the ground state fidelity $F(\lambda_1, \lambda_2)$ for a D-dimensional quantum lattice model onto the partition function of a D-dimensional classical statistical vertex lattice model. This mapping implies that we can take advantage of the whole machinery of the transfer matrix formulation in statistical mechanics. As we discuss below, it also means that we can compute the fidelity per lattice site $d(\lambda_1, \lambda_2)$ by exploiting the TN algorithms of Refs. [17–19].

To establish this mapping, we recall that *any* state of a quantum lattice system may be represented in terms of a TN, such as an MPS for one-dimensional systems or a PEPS for systems in $D \ge 2$ dimensions [14,16]. As a concrete example, let us consider a square lattice on a torus with $N = L_x \times L_y$ sites, where each site, labeled by a vector $\vec{r} = (x, y)$, is represented by a q-dimensional Hilbert space $V^{[\vec{r}]} \equiv \mathfrak{C}^q$. A PEPS for a state $|\psi(\lambda)\rangle$ consists of a set of tensors $A^{[\vec{r}]}$, one tensor per lattice site. Each tensor is made of complex numbers $A^{[\vec{r}]s}_{\alpha\beta\gamma\delta}$ labeled by one *physical* index s and four *bond* indices α, β, γ, and δ (in a generic case, there will be one bond index for each outgoing link of site $\vec{r}$). The physical index s runs over a basis of $V^{[\vec{r}]}$ so that $s = 1, \cdots, q$, whereas each bond index takes Q values, with Q some inner dimension of bonds in the valence bond picture, which connects the tensors in the nearest neighbor sites. In terms of the PEPS representation, the ground state fidelity turns out to be equivalent to the partition function of a two-dimensional classical statistical vertex lattice model, see Fig. 1, with the statistical "weights"

$$E^{[\vec{r}]}_{\tilde{\alpha}\,\tilde{\beta}\,\tilde{\gamma}\,\tilde{\delta}}(\lambda_1, \lambda_2) \equiv \sum_s [A^{[\vec{r}]s}_{\alpha'\beta'\gamma'\delta'}(\lambda_2)]^* A^{[\vec{r}]s}_{\alpha\beta\gamma\delta}(\lambda_1), \tag{3}$$

where the tilded indices are combined pairs of indices: $\tilde{\alpha} \equiv (\alpha, \alpha')$ and so on. By inspecting definitions (1) and (2), one concludes that the logarithm of $d_N(\lambda_1, \lambda_2)$ is formally equivalent to the free energy per site in the two-dimensional classical statistical vertex lattice model [25] (up to an irrelevant prefactor linear in temperature). This argument is valid for any lattice geometry in any dimension [26]. Therefore, the fact that QPTs may be detected as singularities in $d(\lambda_1, \lambda_2)$ matches the conventional wisdom that phase transition points are reflected as singularities, in the thermodynamic limit, of the free energy for classical systems.

Some remarks are in order. First, the mapping is *exact* both for finite lattices (possibly for a large Q) and infinite lattices (infinite Q). Second, for periodic systems that are invariant under translations, one can always build a TN where all the tensors are the same (often at the cost of increasing Q) by using results in [15,27] and generalizations thereof. Finally, in practical computations as described below, the exact ground state is approximated, in a controlled way, by a TN with reasonably small Q.

Fidelity per lattice site from tensor network representations.—From now on, we specialize to a D-dimensional lattice system that is invariant under translations by one

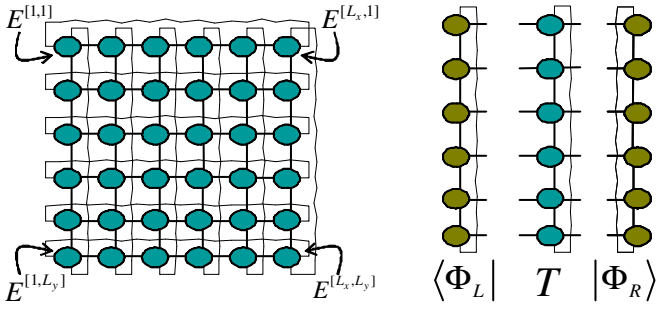

FIG. 1 (color online). Diagrammatical representation of several tensor networks. *Left:* two-dimensional tensor network for the ground state fidelity $F(\lambda_1, \lambda_2)$ in a system defined on a torus. *Right:* matrix product operator (MPO) for the corresponding one-dimensional transfer matrix $T(\lambda_1, \lambda_2)$, and matrix product state (MPS) for the left and right eigenvectors of T, $|\Phi_L\rangle$, and $|\Phi_R\rangle$, with the largest eigenvalue μ.

lattice site [20]. We explain how to obtain the fidelity per site, both in infinite and finite (but large) systems. As a first step, we use the TN algorithms [17–19] to compute a TN representation for the ground states $|\psi(\lambda_1)\rangle$ and $|\psi(\lambda_2)\rangle$ in terms of site-independent tensors $A^{[\vec{r}]}(\lambda_1)$ and $A^{[\vec{r}]}(\lambda_2)$, that we use to build the (also site-independent) statistical weights $E^{[\vec{r}]}(\lambda_1, \lambda_2)$. We notice that all these tensors depend on the lattice size N.

The fidelity $F(\lambda_1, \lambda_2)$, regarded as the partition function of a D-dimensional classical statistical vertex lattice model with weights $E^{[\vec{r}]}(\lambda_1, \lambda_2)$, is the trace of a power of some *transfer matrix* T,

$$F(\lambda_1, \lambda_2) = \mathrm{Tr}(T^{L_x}). \tag{4}$$

Here, T, a $(D-1)$-dimensional tensor network itself, is made of all the tensors $E^{[\vec{r}]}$ contained in some regular slice of the TN for $F(\lambda_1, \lambda_2)$, where the latter consists of exactly L_x identical such slices, see Fig. 1. Let μ_α be the eigenvalues of T, with $|\mu_0| \geq |\mu_1| \geq \cdots \geq |\mu_{\alpha_{\max}}|$. Then, the fidelity reads

$$F(\lambda_1, \lambda_2) = \sum_{\alpha=0}^{\alpha_{\max}} \mu_\alpha^{L_x} = \mu_0^{L_x}\left[1 + \sum_{\alpha=1}^{\alpha_{\max}} \left(\frac{\mu_\alpha}{\mu_0}\right)^{L_x}\right], \tag{5}$$

so that for large L_x, and assuming $|\mu_0| > |\mu_1|$ [28],

$$d_N(\lambda_1, \lambda_2) = \mu_0\left\{1 + O\left[\frac{1}{L_x}\left(\frac{\mu_1}{\mu_0}\right)^{L_x}\right]\right\}. \tag{6}$$

That is, $d_N(\lambda_1, \lambda_2)$ is given by the largest eigenvalue μ_0 of T up to corrections that decay exponentially in the linear system size L_x. Our next task is to determine μ_0, which in general depends on N, λ_1, and λ_2.

First, we compute the left and right eigenvectors $|\Phi_L\rangle$ and $|\Phi_R\rangle$ of T corresponding to μ_0,

$$\langle\Phi_L|T = \langle\Phi_L|\mu_0, \quad T|\Phi_R\rangle = \mu_0|\Phi_R\rangle, \tag{7}$$

where we use a $(D-1)$-dimensional TN to represent them. This is achieved (again with the TN algorithms [17–19]) by exploiting the fact that, e.g., $|\Phi_R\rangle \sim \lim_{p\to\infty} T^p|\Psi_0\rangle$ for an arbitrary state $|\Psi_0\rangle$ such that $\langle\Psi_0|\Phi_R\rangle \neq 0$. After normalizing the states so that $\langle\Phi_L|\Phi_R\rangle = 1$, we obtain μ_0 from

$$\mu_0 = \langle\Phi_L|T|\Phi_R\rangle, \tag{8}$$

by evaluating a $(D-1)$-dimensional TN for $\langle\Phi_L|T|\Phi_R\rangle$, see Fig. 1. At this point, we notice that we can use the techniques that we have just discussed in order to evaluate this new TN, by reducing the calculation to a $(D-2)$-dimensional TN, and so forth.

We illustrate the procedure with two simple cases: (i) periodic chains, $D = 1$; (ii) periodic square lattices, $D = 2$.

Case (i) [29]: Each ground state is represented as an MPS that consists of N copies of the tensor $A^s_{\alpha\beta}$, with one physical index s and two bond indices α and β. The zero-dimensional transfer matrix T is given by $E_{\tilde{\alpha}\,\tilde{\beta}}(\lambda_1, \lambda_2) \equiv \sum_s [A^s_{\alpha'\beta'}(\lambda_2)]^* A^s_{\alpha\beta}(\lambda_1)$, and its diagonalization produces the eigenvalues $\mu_0, \cdots, \mu_{\alpha_{\max}}$.

Case (ii): Each ground state is represented as a PEPS on a torus with $N = L_x \times L_y$ sites, see Fig. 1. The one-dimensional transfer matrix T is a matrix product operator (MPO) with tensors given by the statistical weights $E^{[\vec{r}]}$ of Eq. (3). Its left and right eigenvectors $|\Phi_L\rangle$ and $|\Phi_R\rangle$ with maximal eigenvalue μ_0 are represented as MPSs with tensors $L^s_{\alpha\beta}$ and $R^s_{\alpha\beta}$. The zero-dimensional transfer matrix T' reads

$$T'_{\tilde{\epsilon}\,\tilde{\gamma}} = \sum_{s,s'} (L^s_{\epsilon\gamma})^* E_{\epsilon' s' \gamma' s} R^{s'}_{\epsilon'' \gamma''}, \tag{9}$$

where $\tilde{\epsilon} = (\epsilon, \epsilon', \epsilon'')$ and $\tilde{\gamma}$ are composite indices. Let μ'_0 be the largest eigenvalue of T'. Then, up to corrections that vanish exponentially fast in L_x and L_y, we have

$$F(\lambda_1, \lambda_2) \approx \mu_0^{L_x} = (\mu_0'^{L_y})^{L_x} = (\mu'_0)^N, \tag{10}$$

so that

$$d_N(\lambda_1, \lambda_2) \approx \mu'_0, \qquad d(\lambda_1, \lambda_2) = \mu'_0 \tag{11}$$

for the finite and infinite cases, respectively.

Example: the two-dimensional quantum Ising model with transverse and parallel magnetic fields.—As a test, we compute the fidelity per lattice site $d(\lambda_1, \lambda_2)$ for the two-dimensional quantum Ising model in the thermodynamic limit, as described by the Hamiltonian

$$H = -\sum_{(\vec{r},\vec{r}')} \sigma_z^{[\vec{r}]}\sigma_z^{[\vec{r}']} - \lambda\sum_{\vec{r}} \sigma_x^{[\vec{r}]} - \epsilon\sum_{\vec{r}} \sigma_z^{[\vec{r}]}. \tag{12}$$

Here, $\sigma_x^{[\vec{r}]}$ and $\sigma_z^{[\vec{r}]}$ are the Pauli matrices at the lattice site $\vec{r}$, with the control parameters λ and ϵ being the transverse and parallel magnetic fields. For $\epsilon = 0$, the system has a second order phase transition at $\lambda_c \approx 3.044$ [30], whereas for $\lambda < \lambda_c$, a first order phase transition occurs when ϵ changes sign. We plot $d(\epsilon_1, \epsilon_2)$ and $d(\lambda_1, \lambda_2)$ in Fig. 2, as computed from the infinite PEPS algorithm [18] with bond dimension 2. We can clearly identify the first and second order phase transitions by a discontinuity in $d(\epsilon_1, \epsilon_2)$ and a pinch point in $d(\lambda_1, \lambda_2)$, respectively. The two stable fixed points at $\lambda = 0$ and $\lambda = \infty$ are also characterized as the global minima of $d(\lambda_1, \lambda_2)$.

Summary and outlook.—The fidelity per site $d(\lambda_1, \lambda_2)$ allows us to determine the zero temperature phase diagram of a quantum lattice system without prior knowledge of order parameters. Here, we have shown how to compute $d(\lambda_1, \lambda_2)$ in the context of the TN algorithms of Refs. [17–19]. We envisage that this approach will become a preferred strategy to scan a quantum lattice system for possible phases and phase transitions, perhaps as a first step of a more comprehensive method that will subsequently characterize each phase in terms of order parameters, etc. An interesting question is to see whether or not the scheme works for systems with topological orders. On the other

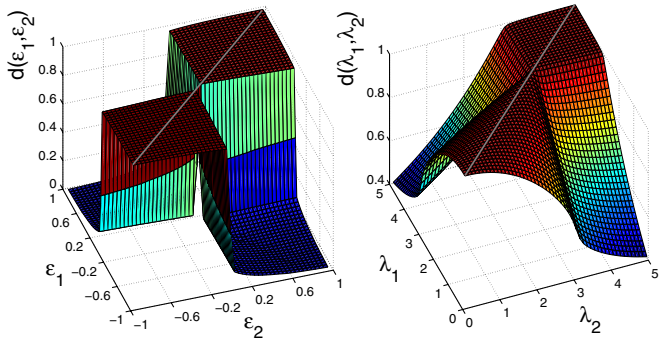

FIG. 2 (color online). Fidelity per lattice site for ground states of the two-dimensional quantum Ising model, Eq. (12), which is one along the diagonal. *Left:* for $\lambda = 2.5$ (i.e., $\lambda < \lambda_c$), $d(\epsilon_1, \epsilon_2)$ displays a discontinuity at the lines $\epsilon_1 = 0$ and $\epsilon_2 = 0$, which indicates the presence of a first order phase transition. *Right:* for $\epsilon = 0$, $d(\lambda_1, \lambda_2)$ has a pinch point at (λ_c, λ_c), indicating the presence of a second order phase transition.

hand, further work is needed to perform finite-size scaling and extract the correlation length critical exponent by exploiting the finite TN algorithms, which is currently under investigation.

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[20] For simplicity, we assume that the system is invariant under translations by one lattice site and that the ground state is represented with a TN that consists of copies of the same tensor. However, it is straightfoward to generalize the present discussion to states that are invariant under translations by some finite number of lattice sites, by considering a TN with the same symmetry.
[21] The extension of our discussion to systems depending on more than one control parameters is straightforward.
[22] Consider a quantum system described by a Hamiltonian $H = H_0 + \lambda H_1$, with $[H_0, H_1] = 0$. Suppose there is a transition point λ_c due to level crossing. Therefore, ground states are the same (orthogonal) if they are in the same (different) phase(s). This implies that $d(\lambda_1, \lambda_2) = 1(0)$ if λ_1 and λ_2 are in the same (different) phase(s). That is, $d(\lambda_1, \lambda_2)$ is discontinuous at $\lambda_1 = \lambda_c(\lambda_2 = \lambda_c)$. This argument may be extended to a general model Hamiltonian with the above situation as a special case.
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[28] The case $|\mu_0| = |\mu_1|$ can also be dealt with by considering the corresponding eigenvectors.
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