Universal construction of order parameters for translation-invariant quantum lattice systems with symmetry-breaking order

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For any translation-invariant quantum lattice system with a symmetry group $G$, we propose a practical and universal construction of order parameters which identify quantum phase transitions with symmetry-breaking order. They are defined in terms of the fidelity between a ground state and its symmetry-transformed counterpart, and are computed through tensor network representations of the ground-state wavefunction. To illustrate our scheme, we consider three quantum systems on an infinite lattice in one spatial dimension, namely, the quantum Ising model in a transverse magnetic field, the quantum spin-$1/2$ XYX model in an external magnetic field, and the quantum spin-$1$ XXZ model with single-ion anisotropy. All these models have symmetry group $\mathbb{Z}_2$ and exhibit broken-symmetry phases. We also discuss the role of the order parameters in identifying factorized states.

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Introduction. In the conventional Landau-Ginzburg-Wilson paradigm a basic notion is spontaneous symmetry breaking, which is traditionally characterized in terms of a local order parameter \[1, 2\]. Typically, such a local order parameter is model-dependent and not always obvious to define. Although attempts have been made to derive a local order parameter for quantum lattice systems undergoing quantum phase transitions (QPTs) \[3, 4\], it is highly desirable to find a simple, unifying, and model-independent way to characterize symmetry-breaking order when it occurs in a quantum lattice many-body system.

In this Letter, we address this issue from a quantum information perspective through the notion of fidelity. In Refs. \[5, 6, 7, 8\], it has been argued that the ground-state fidelity per site may be used to detect QPTs. Since this argument is based solely on a basic postulate of quantum mechanics regarding quantum measurement, the approach is applicable to quantum lattice systems in any number of spatial dimensions, regardless of the type of internal order present in quantum many-body states. It has been confirmed that the ground-state fidelity per site is able to identify QPTs arising from spontaneous symmetry breaking \[5, 6, 7, 8\], the Kosterlitz-Thouless transition \[10\], and topological QPTs in the Kitaev model \[11\]. In an extension of this notion, here we propose a universal approach to define and compute order parameters for any translation-invariant quantum lattice system, with a symmetry group $G$, undergoing a QPT with symmetry-breaking order. We perform the explicit computation of order parameters through the use of tensor network algorithms, in particular the matrix product states (MPS) \[12, 13, 14\] for systems in one spatial dimension.

To illustrate our scheme, we investigate the following models on an infinite lattice in one spatial dimension: the quantum Ising model in a transverse magnetic field, the quantum spin-$1/2$ XYX model in an external magnetic field, and the quantum spin-$1$ XXZ model with single-ion anisotropy. All these systems possess a discrete symmetry group $\mathbb{Z}_2$, which simultaneously broken as the system undergoes a QPT. Although these examples are restricted to $\mathbb{Z}_2$-systems on an infinite-size lattice in one spatial dimension, we emphasize that the scheme extends to any translation-invariant quantum lattice system, with arbitrary symmetry group, in any spatial dimension. For systems in higher spatial dimensions the computation of the ground state is accommodated by the tensor product states (TPS) \[15\], or equivalently, the projected entangled-pair states (PEPS) \[16\].

The construction of these order parameters not only allows us to locate critical points, but also enables us to identify factorized states $|\psi(\lambda_f)\rangle$, where $\lambda_f$ is the so-called factorizing field \[18, 19\]. Such a factorized state $|\Psi(\lambda_f)\rangle$ can occur in the symmetry-broken phase. The fact that no entanglement exists makes it the most ordered state, with a salient feature that the order parameters take their maximum value at $\lambda = \lambda_f$.

Universal construction of order parameters for translation-invariant quantum lattice systems with symmetry-breaking order. Consider an infinite-lattice translation-invariant quantum system with symmetry group $\hat{G}$ and Hamiltonian $H(\lambda)$, with $\lambda$ a control parameter. According to Wigner’s theorem the representations of $g \in \hat{G}$ are either unitary or anti-unitary. The group elements which are represented unitarily form a subgroup $\hat{G} \subseteq \hat{G}$, and we hereafter restrict our considerations to this subgroup. Suppose a symmetry-breaking QPT occurs at a critical point $\lambda_c$ where, without loss of generality, we assume there is no symmetry breaking for $\lambda > \lambda_c$. For the ground state $|\psi(\lambda)\rangle$ in the symmetric phase, the fidelity $\langle |\psi(\lambda)\rangle|g|\psi(\lambda)\rangle\rangle$ is equal to one for any symmetry operation $g \in \hat{G}$. In the broken-symmetry phase $\lambda < \lambda_c$ we have

\begin{equation}
0 \leq \langle |\psi(\lambda)\rangle|g|\psi(\lambda)\rangle\rangle \leq 1,
\end{equation}

where $|\psi(\lambda)\rangle$ and $|\psi(\lambda)\rangle$ are any two states in the degenerate ground state. This description is valid for any system admitting a QPT with symmetry-breaking order, regardless of the type of symmetry group or whether the transitions are continuous or discontinuous. For later use we will denote the
nly occur in the infinite lattice limit, we will utilize an algorithm developed by Vidal [17]. This algorithm provides a representation of the system’s ground-state wavefunction, and in together with two square gates representing a nontrivial element \( g \) of the symmetry group \( G \) acting on physical indices.

Based on this observation we now describe a procedure to construct order parameters which provide quantitative information about symmetry-breaking QPTs. Because QPTs generally occur in the infinite lattice limit, we will utilize an algorithm developed by Vidal [17]. This algorithm provides an efficient way to generate an infinite MPS (iMPS) representation of the system’s ground-state wavefunction, and in turn compute expectation values. Determination of the ground state amounts to computing the imaginary time evolution operator \( \exp(-H\tau) \) acting on an initial state \( |\Psi(0)\rangle \): \( |\Psi(\tau)\rangle = \exp(-H\tau)|\Psi(0)\rangle/\exp(-H\tau)|\Psi(0)\rangle \). In the symmetry-broken phase with ground-state degeneracy, we can obtain more than one ground-state representative through different choices of the initial state \( |\Psi(0)\rangle \). Let \( |\psi(\lambda)\rangle \) and \( |\psi'(\lambda)\rangle \) denote two such iMPS representations (which may or may not be equivalent states). The structure associated to the algorithm, which utilizes the translational invariance of the system, leads to the conclusion that

\[
|\langle \psi(\lambda)|g|\psi'(\lambda)\rangle| = \lim_{L\to\infty} |\text{tr}(E^L)|, \tag{2}
\]

where \( E \), referred to as the transfer matrix, is the four-index tensor schematically defined in Fig. 1 in terms of diagonal singular-value matrices \( \lambda_A, \lambda_B \) and the three-index tensors \( \Gamma_A, \Gamma_B \). The iMPS representation becomes exact in the limit as the dimension of the matrices \( \lambda_A, \lambda_B \) approaches infinity. In practice, we introduce a truncation dimension \( \chi \) associated to \( \lambda_A, \lambda_B \) and adjust \( \chi \) to achieve an extrapolation of results for the \( \chi \to \infty \) case.

Observe next that (2) can only take the values zero or one, since the trace is simply the sum of the eigenvalues. This is in stark contrast to (1), and indicates that the iMPS algorithm is preferential in its convergence to states in the ground-state subspace. Fixing a representative \( |\phi(\lambda)\rangle \), we define \( W_\lambda \) to span \( |\phi_{h}(\lambda)\rangle = h|\phi(\lambda)\rangle : h \in G \). Remembering that the representation of \( G \) is unitary, it also follows that the representation of each \( g \in G \) on \( W_\lambda \) is of the form of a permutation matrix (up to a diagonal unitary transformation). The existence of such a representation for all groups \( G \) follows from Cayley’s theorem, which states that every group is the subgroup of a symmetric group. It may be that \( W_{\lambda} \) does not span the degenerate subspace of the broken symmetry phase. Within the iMPS algorithm, we can generate subspaces orthogonal to \( W_{\lambda} \) simply by choosing the initial state \( |\Psi(0)\rangle \) of the algorithm to be orthogonal to \( W_{\lambda} \). In principle a basis for \( V(\lambda) \) can be constructed in this manner leading to \( V(\lambda) = \mathcal{O}(\lambda)W_{\lambda} \). We then still have that the representation of \( g \in G \) on \( V(\lambda) \), which has a block diagonal structure, is of the form of a permutation matrix.

We can now exploit these facts to uniquely define order parameters which characterize the broken-symmetry phase. For a fixed choice of \( g \in G \) and a fixed iMPS representation \( |\phi(\lambda)\rangle \), let \( f_{g}(\lambda) \) denote the square root of the eigenvalue of \( \Gamma_{g}(\lambda) \) which has the largest absolute value. As such, one sees that \( |f_{g}(\lambda)| = 1 \) for all \( g \in G \) in the symmetric phase \( \lambda > \lambda_c \), and \( 0 \leq |f_{g}(\lambda)| \leq 1 \) in the broken-symmetry phase \( \lambda < \lambda_c \). We now define \( I_{g}(\lambda) \) to be

\[
I_{g}(\lambda) = \sqrt{1 - |f_{g}(\lambda)|^2}. \tag{3}
\]

and argue that the set \( \mathcal{O} = \{ I_{g}(\lambda) : g \in G \} \) defines a set of order parameters which detect QPTs with symmetry-breaking order. First, each \( I_{g}(\lambda) \) is zero if \( \lambda > \lambda_c \). Second, each \( I_{g}(\lambda) \) can take a value ranging from 0 to 1 if \( \lambda < \lambda_c \). These features are nothing but what we require for \( I_{g}(\lambda) \) to be an order parameter. Moreover, \( \mathcal{O} = \{ I_{g}(\lambda) : g \in G \} \) is unique on each block representation \( W_{\lambda} \subseteq V(\lambda) \), that is, in the set is independent of the choice of iMPS representation \( |\phi(\lambda)\rangle \in W_{\lambda} \). To show this, we first consider for each \( G \)-conjugacy class \( C \) the set of order parameters \( \mathcal{O}_{C} = \{ I_{g}(\lambda) : g \in C \} \). Any different iMPS representation \( |\phi'(\lambda)\rangle \in W_{\lambda} \) will be related to \( |\phi(\lambda)\rangle \) by \( |\phi'(\lambda)\rangle = \exp(\phi)|\phi_{h}(\lambda)\rangle \) for some \( h \in G \) and some phase \( \phi \). Due to orthogonality of \( |\phi(\lambda)\rangle \) and \( |\phi'(\lambda)\rangle \), the uniqueness of the set \( \mathcal{O}_{C} \) for \( W_{\lambda} \) follows from

\[
|\langle \phi(\lambda)|g|\phi'(\lambda)\rangle| = |\langle \phi_{h}(\lambda)|g|\phi_{h}(\lambda)\rangle| = |\langle \phi(\lambda)|h^{-1}gh|\phi(\lambda)\rangle|. \tag{4}
\]

Consequently, \( \mathcal{O} = \cup_{C} \mathcal{O}_{C} \) is a uniquely-defined set of order parameters on each subspace block \( W_{\lambda} \subseteq V(\lambda) \). This is in some contrast to the conventional notion of an order parameter, whose value is associated with individual states in \( V(\lambda) \). These considerations are valid for any quantum lattice system where there is symmetry-breaking order, thus the construction can be applied universally. Finally, we define a symmetry-breaking QPT to be second-order if all \( I_{g}(\lambda) \) are continuous functions of \( \lambda \). If there are any discontinuous \( I_{g}(\lambda) \) we say the QPT is first-order.

The models. To illustrate our scheme, we consider three one-dimensional lattice Hamiltonians with \( \mathbb{Z}_{2} \)-symmetry. This group is generated by a single non-trivial element \( g \), which squares to the identity, and in each case admits a unitary

![Transfer Matrix](image-url)
The Hamiltonian takes the form,

$$H = -\sum_{i=0}^{\infty} \left( \frac{1 + \chi}{2} S^x_i S^{x^{i+1}} + \frac{1 - \chi}{2} S^y_i S^{y^{i+1}} + \alpha S^{z}_{i} \right),$$

where $S_{i}^{[\alpha]}$ ($\alpha = x, y, z$) are the spin-1/2 Pauli operators at lattice site $i$, $\chi$ is a transverse magnetic field, and $\gamma$ is an anisotropic coupling constant. The model is invariant under the symmetry operation: $S^z_i \to -S^z_i$, $S^y_i \to -S^y_i$ and $S^z_i \to S^z_i$ for all sites, which yields the $\mathbb{Z}_2$ symmetry. For nonzero $\gamma$, it is critical at $\chi = 1$ [20]. In addition, a factorizing field occurs at $\chi_f = \sqrt{1 - \gamma^2}$. If $\gamma = 1$, the quantum XY model reduces to the quantum Ising model in a transverse field.

We also investigate the quantum spin-1/2 XYX model in an external magnetic field. The Hamiltonian can be written as

$$H = \sum_{i=0}^{\infty} \left( S^{[x]} S^{[x^{i+1}]} + \Delta_{x} S^{[y]} S^{[y^{i+1}]} + S^{[z]} S^{[z^{i+1}]} + h S^{[z]} \right),$$

where $S^{[\alpha]}$ ($\alpha = x, y, z$) are the Pauli spin operators at site $i$, $\Delta_{x}$ is a parameter describing the rotational anisotropy, and $h$ is an external magnetic field. This model also possesses a $\mathbb{Z}_2$ symmetry, with the symmetry operation: $S^x_i \to -S^x_i$, $S^y_i \to -S^y_i$ and $S^z_i \to S^z_i$ for all sites. Below we shall choose $\Delta_{x} = 0.25$. In this case, the critical magnetic field is $h_{c} \sim 3.210(6)$ \cite{18}, with a factorizing field $h_{f} \sim 3.162$.

The last model considered here is the quantum spin 1 XXZ model with single-ion anisotropy. The Hamiltonian takes the
Form,\[ H = \sum_{i=0}^{\infty} \left[ J_i S_x^{(i)} S_x^{(i+1)} + S_y^{(i)} S_y^{(i+1)} + J_z S_z^{(i)} S_z^{(i+1)} \right] + D \sum_{i=0}^{\infty} S_z^{(i2)}, \] where \( S_\alpha^{(i)} (\alpha = x, y, z) \) are the spin-1 operators at the \( i \)-th lattice site, \( D \) represents uniaxial single-ion anisotropy. We choose \( J = 1, J_z = 10 \), with \( D \) as the control parameter. As such, the system undergoes a first-order QPT from a gapped \( \mathbb{Z}_2 \) symmetry-broken Néel phase to a gapped \( \mathbb{Z}_2 \) symmetric large-\( D \) phase, with the symmetry operation: \( S_x^{(i)} \to S_x^{(i)} \), \( S_y^{(i)} \to -S_y^{(i)} \) and \( S_z^{(i)} \to S_z^{(i)} \) for all sites.

The results. In Fig.2 we plot the universal order parameter \( I(\lambda) \) for the quantum Ising model in a transverse field, with the field strength \( \lambda \) as the control parameter. For the control parameter \( \lambda \) less than a pseudo critical value \( \lambda_c \), the universal order parameter \( I(\lambda) \) is non-zero, which characterizes the \( \mathbb{Z}_2 \) symmetry-broken phase. In the symmetric phase \( \lambda > \lambda_c \), the universal order parameter \( I(\lambda) \) is zero. When the control parameter \( \lambda \) varies across the point \( \lambda_c \), the behavior of the universal order parameter \( I(\lambda) \) implies that the system undergoes a phase transition at the \( \lambda_c \). As the truncation dimension \( \chi \) is increased, \( \lambda_c \) moves toward the known critical point \( \lambda_c = 1 \). Performing an extrapolation of \( \lambda_c \) with respect to \( \chi \), we obtain \( \lambda_c = 1.0023 \). Note that the universal order parameter reaches the maximum value at \( \lambda = 0 \). The maximum value of \( I(\lambda) \) coincides with the existence of a factorized state at this point, in which no entanglement exists.

In Fig.3 the universal order parameter \( I(\lambda) \) for the quantum spin 1/2 XY model in an external magnetic field \( \lambda \) is plotted, with the magnetic field strength \( \lambda \) as the control parameter. A transition point \( \lambda_t \) occurs as \( I(\lambda) \) varies from zero to nonzero values. With increasing truncation dimension the transition point \( \lambda_t \) approaches the critical point \( \lambda_c = 1 \). Performing an extrapolation with respect to \( \chi \) yields the critical point \( \lambda_c = 1.000039 \). A factorizing field \( \lambda_f \) occurs at \( \lambda_f = 0.5 \), where again \( I(\lambda) \) takes its maximum value.

In Fig.4 we show the universal order parameter \( I(h) \) between a ground state and its symmetry-transformed counterpart for the quantum XXZ model in an external magnetic field. In the range \( h < h_c \), the universal order parameter \( I(h) \) is non-zero, which characterizes the \( \mathbb{Z}_2 \) symmetry-broken phase. A transition point \( h_t \) occurs as \( I(h) \) vanishes. As the truncation dimension \( \chi \) increases, the transition point \( h_t \) approaches the critical point \( h_c = 3.2052 \). Performing an extrapolation of \( h_t \) with respect to \( \chi \), we obtain \( h_c = 3.2052, a = 0.0277, b = 0.9848 \). The universal order parameter \( I(h) \) takes the maximum value at \( h_f \sim 3.16 \).

In Fig.5 the universal order parameter \( I(D) \) is plotted for the quantum XXZ model with single-ion anisotropy. For \( D < D_c \), the system is in the gapped \( \mathbb{Z}_2 \) symmetry-broken Néel phase, so the universal order parameter \( I(D) \) is nonzero. For \( D > D_c \), it is in the gapped \( \mathbb{Z}_2 \) symmetric large-\( D \) phase, so \( I(D) \) is zero. We see that \( I(D) \) is discontinuous, providing an example of a first-order QPT. As the truncation dimension \( \chi \) increases, the transition point \( D_t \) approaches the critical point \( D_c = 9.9434 \).

Summary. We have described a universal procedure to compute order parameters for any translation-invariant quantum lattice system with a symmetry group \( G \). The scheme has been illustrated for the quantum Ising model in a transverse magnetic field, the quantum spin-1/2 XY model in an external magnetic field, and the quantum spin-1 XXZ model with single-ion anisotropy, by exploiting the infinite MPS algorithm for one-dimensional systems. In all instances the procedure is successful in identifying the QPT points. Moreover, we observe that occurrences of factorizing fields are in correspondence with the maximal values of the order parameters.

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