Local indistinguishability and edge modes revealed by the sub-system fidelity

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Abstract

We propose to use the sub-system fidelity, defined by comparing a pair of reduced density matrices, to identify and locate zero modes relating two degenerate ground states in one-dimensional interacting many-body systems, where the degeneracy arises from either symmetry protected topology (SPT), or from discrete symmetry breaking (DSB). A theorem is provided to construct locally indistinguishable (LI) states by linear recombination of the degenerate states of minimal bulk entanglement entropy. The theorem enables us to construct local operators that swap exactly the LI states and are therefore the zero energy modes in the many-body system. Interestingly, they can be located anywhere in the DSB case, but can only be accommodated near the edges in the SPT case. This can be used to identify or distinguish SPT states against the so-called cat states in the DSB case. We illustrate the results for the anisotropic Haldane chain and the interacting Kitaev model.

1. Introduction

Traditional states of matter are characterized by local order parameters in the framework of Landau’s theory of symmetry breaking [1]. However, topological states of matter have no characteristic local order parameters but are topologically non-trivial [2]. Such states are said to support topological orders. In terms of ground state entanglement, they fall into two categories. The first is the intrinsic topological order [3], which has long-range entanglement. It can be characterized by the ground state degeneracy on closed manifolds and the fractional statistics between quasi-particle excitations [4–6]. The second is the symmetry protected topological (SPT) order [7] where the entanglement is only short-ranged. It is a generalization of the topological insulators (TI) and topological superconductors (TSC) [8, 9], and can be characterized by zero edge modes on open boundaries [10–12].

Recently, the diagnosis of SPT states in low dimensions has attracted much attention. One strategy is to use the topological quantity constructed from the bulk states. For example, for non-interacting fermionic systems, topological indices such as the Chern number [13] and \(Z_2\) index [14] can be constructed from bulk energy bands and a complete classification has been developed [15]. However, it was found later that the classification based on non-interacting topological indices may become invalid in the presence of interactions [16, 17]. In such cases the degeneracy in the entanglement spectrum was proposed as an indicator of the non-trivial topology in the bulk wave functions [18, 19]. Meanwhile, by applying matrix-product representation of the wave function, one dimensional SPT phases were shown to be classified by projective representations of symmetries [20–22]. A more recent scheme is the so-called ‘strange correlator’ [23, 24], which saturates to a constant or decays algebraically if the detected states host non-trivial short-range entanglement. Another way is to detect the non-trivial zero edge modes on open boundaries directly, utilizing the bulk-edge correspondence. In fact, most practical experimental set-ups [25] follow this line since the edge modes are directly measurable. From a theoretical point of view, the implementation of this idea is rather obvious for non-interacting fermionic systems because the exact wave function of every single-particle mode can be obtained by solving the single-particle Schrödinger equation. In an interacting system, the ground state degeneracy in open boundary
conditions implies edge degeneracy [26], but the structure of the edge mode necessarily goes beyond the single-particle picture, and is not yet clearly understood.

Interesting clues come from the studies of the difference between degenerate ground states in terms of local measurements. It is found that topologically degenerate ground states are locally indistinguishable (LI) and can be transformed into each other by operators confined in a restricted region [27, 28]. In a variational way, a local operator can be constructed by minimizing its spatial range and yet maximizing the difference between its expectation values in the degenerate states (or reduced density matrices of a subsystem containing the measured region) [29, 30]. Very naturally, in the symmetry breaking case, this operator serves as the local order parameter. In the topological case, however, the degenerate ground states cannot be distinguished by any local operator but by nonlocal operators defined on areas with nontrivial topologies [29].

While the above studies were aimed at intrinsically topological systems where ground state degeneracy occurs on closed manifolds, here we extend the concept of LI to SPT systems where degeneracy only arises due to open boundaries. The motivation is to look for (or construct) LI states and the local operators that swap such states. The latter can be naturally interpreted as the zero energy modes. Notice that, because of the boundaries, the degenerate states are no longer necessarily LI, even in the SPT case. In fact the construction of LI states is one of the main points in this work. For our purpose, we utilize the sub-system fidelity (SSF) [31], defined by comparing a pair of reduced density matrices derived from the degenerate ground states, to characterize the local indistinguishability and construct the edge modes in one-dimensional interacting many-body systems.

We remark that the SSF is measurement independent yet represents the minimal statistical overlap achievable by a positive operator-valued measurement (POVM). This avoids the variational search of an optimal local order parameter, e.g., in [29]. In fact the SSF can be calculated straightforwardly in the framework of a matrix product state (MPS). We limit ourselves to ground state degeneracy arising from either SPT or from discrete symmetry breaking (DSB).

The main results of this work are as follows. We provide a theorem to obtain LI states in terms of SSF by linear recombination of the degenerate states, for both SPT and DSB cases. This enables us to construct zero energy modes, or local operators that exactly swap the LI states. They can be located anywhere in the DSB case, but can only be accommodated near the edges in the SPT case. We also show that a nonlocal measurement of the two edges can distinguish the SPT states but not the cat states (the symmetry-protected states in the DSB case) unless the entire chain is involved in the measurement. This provides a scheme to identify/distinguish SPT and DSB, even if the ground states are (or are made to be) eigenstates of the underlying discrete symmetry. We illustrate the results for the anisotropic Haldane chain and the interacting Kitaev model.

The rest of the paper is organized as follows. In section 2, we introduce the basic idea of SSF, provide a theorem to construct LI states and subsequently present a concrete scheme to construct zero energy modes. Section 3 illustrates the application to two concrete models. Section 4 provides a summary and some perspective remarks.

2. Sub-system fidelity, local indistinguishability and zero modes

2.1. Definition

The fidelity $F$ between two ensembles $X_1$ and $X_2$ described by the density matrices $\rho_1$ and $\rho_2$, respectively, is defined as [31],

$$F = \text{Tr} \sqrt{\rho_1^\dagger \rho_2 \sqrt{\rho_1^\dagger}}. \quad (1)$$

When $X_1$ and $X_2$ are pure ensembles, $F$ reduces to the norm of the inner product of the two corresponding quantum states. If $F = 1$, the expectation values of any observable with respect to $\rho_1$ and $\rho_2$ are identical. Thus it is the natural generalization of the inner product between two quantum states and measures the overlap of two ensembles: the two ensembles are ‘orthogonal’ or completely distinguishable if $F = 0$, and ‘identical’ or indistinguishable if $F = 1$.

A strong statement can be made for the case of $F = 0$. Suppose in the respective diagonal basis, for $\mu = 1, 2$, $\rho_\mu = \sum_{i=1}^{N_\mu} A_i^{\mu} \langle \mu | i \rangle \langle i | \mu \rangle$, where $N_\mu$ is the number of nonzero (and positive) eigenvalues of $\rho_\mu$, we obtain

$$F = \text{Tr} \sqrt{\rho_1^\dagger \rho_2} = \sum_{i=1}^{N_1} \lambda_i, \quad \text{where } \mathcal{O} \text{ is the overlap matrix with the components } \mathcal{O}_{ij} = A_{i1} A_{j2} \langle i | j \rangle,$$

and $\lambda_i \geq 0$ is an eigenvalue of the positive semi-definite hermitian operator $\mathcal{O}^\dagger \mathcal{O}$. We observe that $F = 0$ implies $\lambda_1 = 0$ so that $\sum_{i=1}^{N_1} \lambda_i = \text{Tr} \mathcal{O}^\dagger \mathcal{O} = \sum_{i=1}^N |\mathcal{O}_{i1}|^2 = 0$. This is possible if and only if $\mathcal{O} = 0$. Since $A_{i\mu}$ is nonzero, this implies $\langle i | j \rangle = 0$. We conclude that if $F = 0$ for two density matrices, the nonzero-eigenvalued eigen states of these matrices are all orthogonal. In other words, $\{|i1\rangle\}$ and $\{|j2\rangle\}$ span two mutually orthogonal subspaces. We will refer to this statement as the orthogonality lemma.

In the following we will consider the reduced density matrix for a pure state $|\psi\rangle$. As usual, it is obtained by partitioning the system into two parts, say the sub-systems $M$ and $\overline{M}$, and then tracing out the degrees of
freedom of the environment part \(\hat{M}\): \(\rho_M = \text{Tr}_{\hat{M}}|\psi\rangle\langle\psi|\). We obtain two reduced density matrices for two degenerate states, respectively. The resulting fidelity, which we call SSF, depends on the sub-system holding the reduced density matrix. It tells to what extent the two states are indistinguishable by measurements within the given sub-system. Numerically we obtain the SSF for arbitrary segments of a chain efficiently on the basis of MPS, avoiding the explicit form of reduced density matrices (see the appendix for more details).

2.2. Polar states and locally indistinguishable states

We consider two orthogonal quantum states \(|N\rangle\) and \(|S\rangle\) in a \(d\)-dimensional space. Suppose these states can be distinguished in disconnected local regions \(X_i, i = 1, 2, \cdots, I\), in the sense \(F_{NS}^{X_i} = 0\), where and henceforth the subscripts indicate the two states under comparison and the superscript indicates the subsystem for the reduced density matrices. We may form linear recombinations of \(|N\rangle\) and \(|S\rangle\) as

\[
|\psi\rangle = \cos \frac{\theta}{2} |N\rangle + \sin \frac{\theta}{2} |S\rangle, \tag{2}
\]

where \(\theta\) and \(\phi\) are Euler angles. They can be mapped onto the so-called Bloch sphere, as illustrated in figure 1, with \(|N\rangle\) and \(|S\rangle\) the polar states at the north and south poles, respectively.

In practice, if the parity (or \(Z_2\) symmetry) in our context is not enforced, the density matrix renormalization group (DMRG) in a finite system always provides a symmetry-breaking ground state having minimal entanglement entropy. Such states are natural candidates for the polar states. On the other hand, if the symmetry is enforced in the DMRG, the ground state is automatically symmetrical or antisymmetrical under the symmetry operation. In this case, it is straightforward to find the polar states by the recombination and subsequent minimization of entanglement. At this point, the following development applies in both cases.

As will become clearer, there is a fundamental difference between zero modes in SPT and DSB states. The zero modes are most conveniently constructed through the maximally LI states. We therefore state a theorem on how such LI states can be obtained from polar states: Any two states on the equator of the Bloch sphere spanned by \(|N\rangle\) and \(|S\rangle\) are indistinguishable unless all \(X_i\) are jointly measured. The theorem is proved as follows.

We divide the system as \(\Omega = M \cup \hat{M}\) and assume the measurement is performed in the subsystem \(M\). The theorem holds trivially if all \(X_i\) are within \(M\). To make a general case, we assume some of \(X_i\) are in \(M\) and the others in \(\hat{M}\), so that \(F_{NS}^{X_i} = F_{NS}^{M,\hat{M}} = 0\). We perform a Schmidt decomposition

\[
|N\rangle = \sum_n w_n |n_M\rangle |n_{\hat{M}}\rangle, \quad |S\rangle = \sum_s v_s |s_M\rangle |s_{\hat{M}}\rangle,
\]

where and henceforth \(w_n = 0\) and \(v_s = 0\). The reduced density matrices in the subsystem \(M\) are, correspondingly,
\[ \rho_N = \sum_n |w_n|^2 |\eta_n\rangle \langle \eta_n|, \quad \rho_S = \sum_s |v_s|^2 |\sigma_s\rangle \langle \sigma_s|. \]

Since \( F^M_{N,S} = 0 \), by the orthogonality lemma we know that \(|\eta_N\rangle\) and \(|\eta_M\rangle\) are orthogonal. By the same token, \(|\eta_{NS}\rangle\) and \(|\eta_{LR}\rangle\) are also orthogonal. As a result, the reduced density matrix for an arbitrary state \(|\psi\rangle\) defined above must be block-diagonal in the subspaces spanned by \(|\eta_N\rangle\) and \(|\eta_M\rangle\),

\[ \rho_\psi = \cos^2 \frac{\theta}{2} \rho_N + \sin^2 \frac{\theta}{2} \rho_S. \]  

This is an analogue of the expansion of wave functions in terms of their orthogonal bases, and applies equally well to the reduced density matrix of any other state \(|\psi'\rangle\) characterized by Euler angles \( (\theta', \phi') \). Given the block-diagonality, the fidelity between \( \rho_\psi \) and \( \rho_\phi \) is just a summation over that in each subspace, and the result is

\[ F^M_{\psi,\phi'} = \cos \frac{\theta - \theta'}{2}, \]

where we used the fact that \( \text{Tr} \rho_{N,S} = 1 \). Now if \(|\psi\rangle\) and \(|\psi'\rangle\) are both on the equator of the Bloch sphere, namely, \( \theta' = \pi - \theta = \pi/2 \), the fidelity is unity so that any two such states can not be distinguished by measurements in the region \( M \). (The fidelity would be super-unity for any \( \theta = \theta' \), but orthogonality between \(|\psi\rangle\) and \(|\psi'\rangle\) requires \( \theta' = \pi - \theta \). This finishes the proof of the theorem.

We now specialize to the case of open chain, with \( \Omega = L \cup R \), where \( L \) and \( R \) denote the left and right parts, respectively. Suppose \( F^L_{\psi,N}(l \geq \lambda_L) = 0 \) and \( F^R_{\psi,N}(l \geq \lambda_R) = 0 \), where \( l \) indicates the size of the given subsystem and \( \lambda_L, \lambda_R \) is the minimal size of the distinguishable region. We consider two orthogonal states on the equator,

\[ |\phi^+\rangle = \frac{\sqrt{2}}{2} (|N\rangle \pm e^{i\phi}|S\rangle). \]

By the above theorem, we have

\[ F^L_{\phi^+,\phi'} (l \leq N - \lambda_L) = 1, \quad F^R_{\phi^+,\phi'} (l \leq N - \lambda_R) = 1, \]

where \( N \) is the total size of the open chain. This means that \(|\phi^+\rangle\) and \(|\phi^-\rangle\) are LI in the bulk (if \( \lambda_{L,R} \) is finite).

### 2.3. Zero modes and edge modes

Next, we show how to construct operators that can flip the LI states exactly. For degenerate states, such operators represent zero modes. We will show that the behavior of the zero modes is fundamentally different in the SPT and DSB cases.

To construct the zero mode at the left edge, we consider a sub-system \( L \) of minimal size \( \lambda_L \) and its complementary set \( R \) such that \( F^L_{N,S} = F^R_{N,S} = 0 \). We can then define an operator in \( L \),

\[ \hat{O}_L = \sum_n |n_L\rangle \langle n_L| - \sum_s |n_S\rangle \langle n_S|. \]

By orthogonality between \(|n_L\rangle\) and \(|n_S\rangle\), we find \( \hat{O}_L |\phi^+\rangle = |\phi^+\rangle \). This is therefore exactly the zero mode between the two degenerate and LI states. Similarly, we can construct the zero mode at the right edge by minimizing \( R \). When the zero mode operators are coupled to a bias field, they break the ground state degeneracy most efficiently [32]. Notice that the minimal subsystem size is directly obtainable from the size dependence of the SSF, as we will show in the next section.

If the left and right edges are the only distinguishable regions for \(|N\rangle\) and \(|S\rangle\), the above construction provides the genuine edge zero modes. This is the case for the SPT states since these states are gapped and indistinguishable in bulk. The situation is different for the DSB case, where the symmetry-preserving LI states are usually referred to as cat states, and the polar states \(|N\rangle\) and \(|S\rangle\) are distinguishable everywhere because of the local order parameter. We may use any sub-system \( M \) in the interior of the chain and the complementary set \( \bar{M} \) in place of \( L \) and \( R \), respectively. We then have \( F^M_{N,S} = F^N_{M,S} = 0 \), and we can repeat the above arguments to find a zero mode operator in \( M \) of minimal size. Because the location of \( M \) is arbitrary, the zero mode can be located anywhere. This is a fundamental difference to the SPT case, and for this reason the cat states are not topological.

### 3. Applications

#### 3.1. Spin-1 chain

In this subsection we apply our strategy to the spin-1 chain described by the Hamiltonian [18]

\[ H = \sum_i J \vec{S}_i \cdot \vec{S}_{i+1} + U_{zz} (S^z_i)^2. \]

For an anti-ferromagnetic coupling \( J > 0 \) and a positive \( U_{zz} > 0 \), this model has two phases: when \( U_{zz} \) is small, the model is in the Haldane phase, which is a topologically non-trivial phase protected by the time reversal symmetry, or the dihedral group of \( \pi \) rotations about two orthogonal axes, or bond centred inversion symmetry;
when $U_{zz}$ is large, the model is in an anti-ferromagnetic (AFM) phase which breaks the $Z_2$ symmetry that flips the $z$ component of the spin operator.

We obtain the ground state of this model by the DMRG simulations [33, 34]. In the calculation, we consider a system with a total number of sites up to $N = 120$ and keep up to $m = 80$ states in the DMRG block with more than five sweeps to get converged results. The truncation error is of order $10^{-9}$ or smaller.

In the open boundary condition, the Haldane phase is 4-fold degenerate, which can be understood by the existence of one isolated spin 1/2 on each end of the chain. Excluding the identical gaped interior part, these four states can be represented as $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$. Out of these states, $|\uparrow\uparrow\rangle$ lies in the $S_z = 1$ sector, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ in the $S_z = 0$ sector. We consider a sub-manifold with conserved $S_z = 0$. Apparently, $|N\rangle = |\uparrow\downarrow\rangle$ and $|S\rangle = |\downarrow\uparrow\rangle$ can be distinguished by measurements on either edge because the expectation values of the local operator $S_z$ acting on either end of the chain in these two states are different. Thus these two states define the polar states on the Bloch sphere. A pair of orthogonal states can be formed as $|\psi\rangle = \cos \frac{\theta}{2} |N\rangle + e^{i\phi} \sin \frac{\theta}{2} |S\rangle$ and $|\psi^\prime\rangle = \sin \frac{\theta}{2} |N\rangle - e^{i\phi} \cos \frac{\theta}{2} |S\rangle$. The SSF $F^L$ between $|\psi\rangle$ and $|\psi^\prime\rangle$ is shown as a function of the subsystem size $l$ in figure 2(a), for $\theta = 0$, $\pi/4$ and $\pi/2$. (The SSF is independent of the azimuthal angle $\phi$.) In the polar case ($\theta = 0$), $F^L(l)$ drops to zero quickly as $l$ exceeds a characteristic length. To have a better view of the drop of $F^L(l)$, we define an edge profile $f(l) \equiv [F^L(l - 1)]^2 - [F^L(l)]^2$ with the boundary condition $F(l \leq 0) = 1$. Notice that $f(l) \geq 0$ and satisfies the sum rule $\sum f(l) = 1$. The edge profile is shown in the inset of figure 2(a). For the states on the equator ($\theta = \pi/2$), $F^L(l)$ is initially unity and drops to zero only if $l \sim N$ such that the sub-system includes the two edges. This means the pair of states on the equator are indistinguishable unless a measurement involving both edges is performed. These pairs of states can be considered as the Bell entangled states of the edge modes [35]. The bulk entanglement spectrum in the polar states are identical since they are related by $Z_2$ symmetry. Therefore, the equator states are at least 2-fold degenerate in the entanglement spectrum, as is clear from equation (4). Their entanglement Shannon entropies are larger by one unit than those in the polar states. Such characteristics can be used to geometrically represent the polar states from the equator states. For a general $\theta$ on the Bloch sphere, $F^L(l)$ drops from unity initially, saturate at $\sin \theta$ as $l$ is in the bulk, as equation (5) implies, and drops to zero when the right edge is approached. This is exemplified by the case of $\theta = \pi/4$. All of the above behaviors are also observed if we consider $F^R(l)$, with the understanding that the sub-system starts from the right edge and expands (as $l$ increases) toward the left edge.

In the AFM phase, the ground state is 2-fold degenerate. We use $|N\rangle = |+\rangle$ and $|S\rangle = \{-\}$ to represent the two polar states of opposite Neel orders. They are apparently distinguishable at any site. A general pair of orthogonal states $|\psi\rangle$ and $|\psi^\prime\rangle$ are formed similarly to the above case, characterized by the Euler angles $(\theta, \phi)$. As shown in figure 2(c), $F^L(l)$ behaves similarly to that in (a) for all cases of $\theta$. Notice the pair of states with $\theta = \pi/2$ are just the cat states. The edge profile for the polar states $(\theta = 0)$ is shown in the inset.

Although $F^L$ captures the features of the edge, it fails to tell the difference between the SPT and AFM cases. To have a better resolution, we consider another kind of SSF: $F^C(l)$ for a sub-system $C = L \cup \Omega$ out of $\Omega = L \cup C \cup R$, where the size is $l/2$ in both $L$ and $R$. The corresponding results are shown in figures 2(b) and (d). For the Haldane phase in (b), $F^C(l)$ drops to zero quickly for all cases of $\theta$, implying that the states can be distinguished immediately by non-local measurements involving both edges. For the polar states $(\theta = 0)$, this is obvious since different spin moments are present on the edges. For equator states $(\theta = \pi/2)$, the edge spins form either a singlet or a triplet, and this is distinguishable if both edges are simultaneously measured. The states with $\theta = \pi/4$ lie in-between the two extremes and thus behave accordingly. For the AFM phase in (d), $F^C(l)$ also drops quickly for the polar states $(\theta = 0)$, since the latter states are distinguishable everywhere by local order.

Figure 2. Square of the SSF versus the sub-system size $l$ for a pair of degenerate ground states (characterized by $\theta$) in the Haldane phase, with $U_{zz} = 0$ ($U_{xx} = 1/2$) in the upper (lower) panels. (a) and (c) are the square of the SSF in the subsystem $L$, with the insets showing the edge profile. (b) and (d) are the square of the SSF in $C = L \cup R$ out of $\Omega = L \cup C \cup R$. 

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parameters. In contrast to the SPT states, however, the equator states \( (\theta = \pi/2) \) can not be distinguished in \( \hat{C} \) unless \( l \approx N \). This is somehow counter-intuitive, but fully consistent with our theorem: if the measurement does not include the entire chain, there are always remaining distinguishable segments in the environment parts of \( |N \rangle \) and \( |S \rangle \) for the AFM phase, and therefore the equator states are indistinguishable. Therefore \( F^C(l) \) for the equator states is able to distinguish SPT states from cat states.

Having characterized the SPT and AFM phases separately, we now discuss how they are transformed into each other as the control parameter \( U_{zz} \) varies in a physical system. The results are presented in figure 3. Here, we define the penetration depth of an edge profile as \( \xi = \sum_l |f(l)|^2 \). From \( |F^l(l)|^2 \) for polar states in (a) we extract \( \xi \) and plot it versus \( U_{zz} \) in (b). Similarly, from \( |F^C(l)|^2 \) for equator states in (c) we extract a penetration depth \( \tilde{\xi} \) and plot it in (d).

With the increase of \( U_{zz} \), \( \xi \) decreases slightly but remains finite, being insensitive to the transition from SPT to AFM. This is because the polar states are distinguishable on either edge for both cases of SPT and AFM. However, \( \tilde{\xi} \) is finite for small \( U_{zz} \) (where the system is in the SPT phase and the equator states are distinguishable by and only by the nonlocal measurement of both edges), and saturates to the order of \( N \) as \( U_{zz} \gg 1/4 \) (where the AFM phase renders the equator states indistinguishable unless the entire system is measured, see the previous section). This transition point is in agreement with that found in [22]. Therefore \( \tilde{\xi}/N \to 0 \) (or 1) is a useful indicator of the SPT (or symmetry breaking). We check how this corresponds to the distribution of the average local moments. As shown in figure 3(e), (in the polar states) the local moments appear only at the edge in the Haldane phase where \( U_{zz} \ll 1/4 \), while they appear everywhere in the AFM phase where \( U_{zz} > 1/4 \). With increasing \( U_{zz} \ we show a gradual penetration of local moments from the edge to the bulk. In figure 3(f), we show the local moments at the two central sites (the black solid line) and the net magnetic moment in the left half of the chain (the red dashed line). (The expectation values are identical, up to a minus sign, in each pair of orthogonal and degenerate states.) Just as expected, the AF moment develops a non-zero value around \( U_{zz} \approx 1/4 \), and at the same time the net magnetic moment is about 1/4 (half way between zero and half spin). These results indicate a transition point \( U_{zz} \approx 1/4 \), in agreement with that determined by \( \tilde{\xi}/N \).

3.2. Interacting the Kitaev chain and the XZ spin model

The Kitaev chain [36] describes spinless fermions with \( p \)-wave pairing in one dimension. The original Kitaev model is free from interaction. Here we incorporate interaction to investigate the many-body effects. The Hamiltonian is

\[
H = \sum_i \left( t c_i^\dagger c_{i+1} + \Delta c_i^\dagger c_{i+1}^\dagger + \text{h.c.} \right) - \mu \sum_i c_i^\dagger c_i + V \sum_i (n_i - 1/2)(n_{i+1} - 1/2).
\]

Figure 3. Numerical results in the \( S_z = 0 \) sector for a range of \( U_{zz} \) indicated in the legend. (a) \( F^l(l) \) (squared) for polar states. (b) The penetration depth \( \xi \) of the edge profile determined from (a). (c) \( F^C(l) \) (squared) for equator states. (d) The penetration depth \( \tilde{\xi} \) determined from (c), plotted as \( \tilde{\xi}/N \). (e) The anti-ferromagnetic moment on the chain. (f) The anti-ferromagnetic moment (black solid line) on the central two sites of the chain and the net magnetic moment (red dashed line) in the left half of the chain.
transformation, the model can be mapped to an XZ spin model,

\[ H = \sum_i (J_x S_x^i S_x^{i+1} + J_z S_z^i S_z^{i+1} - h S_z^i), \]  

with \( J_x = 4t, J_z = V \) and \( h = \mu \).

The ground states of these two models are determined by the DMRG simulations in a similar setting described above. In the calculation of the SSF in the Kitaev model, we always bring the target sub-system to the left of the environment to avoid the fermion sign caused by the environment. (The fermion sign within each sub-system is retained rigorously.)

By correspondence, the topological phase of the Kitaev model is mapped to the \( Z_2 \) AFM phase (the \( S_z \)-ordered phase) of the XZ model. The latter was often argued to also host Majorana zero modes in the literature [37–39]. However, since the Jordan–Wigner transformation is non-local, the physics of these two phases is rather different, even though they are mathematically equivalent [40]. For symmetry breaking (polar states) and symmetry preserving states (equator states), these two phases show exactly the same features in \( F^2 \) (see figure 4) due to their mathematical equivalence. However, differences take place when measurements are performed on both edges by tracing out \( \sigma \) in favour of \( F^2 \) (l). With moderate \( l \) in the right panels of figure 4, it is shown that the cat states \( (\theta = \pi/2) \) in the XZ model are indistinguishable, as shown in (d), while the SPT states \( (\theta = \pi/2) \) in the Kitaev model can certainly be distinguished, as shown in (b). The underlying reason for the above results is the presence/absence of local order parameters in the bulk, as we discussed for the spin-1 Heisenberg model. As we pointed out in section 2.2, zero energy excitation can be located within any continuous segment in the symmetry-breaking phase, such as that in the XZ model. In this sense, we believe it is improper to call the edge operators in the XZ model as genuine edge modes, although they could be mapped to Majorana operators through Jordan–Wigner transformation. In fact, if the fermion sign in the Kitaev model were ignored in the analysis of the (true) ground states, we would get exactly the same SSFs for both models.

4. Summary

Utilizing the SSF, we proved both analytically and numerically that degenerate symmetry preserving states (equator states) in one-dimensional models are LI states, in both the SPT and DSB cases. These states can be constructed from a linear combination of the polar states that are maximally distinguishable in terms of the SSF. We then provided explicit construction of zero energy modes that swap exactly the LI states. The zero mode can be located anywhere in the DSB phase, while it can only be located at the edges in the SPT case. This provides a novel scheme to differentiate SPT states from cat states of the DSB. We illustrated the results in the anisotropic spin-1 Haldane chain and the interacting Kitaev models. The SSF is not only useful to reveal the properties of the edge modes in interacting SPT systems, but is also able to reveal the evolution from the DSB phase to SPT phase as the control parameter varies.

Our theorem regarding LI states is general and applicable in higher dimensions. The SSF can be defined with respect to any two many-body states, and hence can be defined equally well for excited states. It remains to be seen what could be achieved from such extensions, e.g., in the context of many-body localization. Finally, in this work the SSF is applied to SPT systems where the ground state degeneracy arises from open boundaries. On closed manifolds the SPT ground state is nondegenerate. However, in intrinsically topological systems,
degeneracy occurs even on closed manifolds, and it is an interesting future topic to see how SSF could be used to characterize the properties of such states.

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Appendix

Here we describe in some detail the calculation of the SSF for any two states $|\psi\rangle$ and $|\psi'\rangle$. Assuming $\Omega = L \cup R$, we want to compare the states in the subsystem $L$. We assume that the corresponding reduced density matrices $\rho$ and $\rho'$ are in the form of equation (3) in the main text. The SSF is then expressible as $\rho = \rho'$, where the overlap matrix is defined by $\rho = \langle w |\psi \rangle (\psi | w \rangle$. Numerically we keep the MPS right canonical, namely, the states in $R$ form an orthonormal set. A final singular-value decomposition $\rho = U S V$ enables us to write $\rho = V S V$. Notice that $\rho$ depends on the states under comparison as well as the size $l$ of the subsystem $L$.

However, the evaluation of the overlap matrix becomes tricky for $\rho = \rho'$, where $\rho = \rho'$ out of $\Omega = L \cup C \cup R$. The difficulty is to make the states in the environment block $C$ orthonormal. The idea is to get a mixed state by tracing out the environment $C$. In the first stage, we get the outer product for the environment block

$$E_{a | \alpha} = \sum_{\alpha} \langle \sigma | \psi\rangle \langle \psi | \sigma \rangle_{a | \alpha}$$

where $\psi_{a | \alpha}$ is the matrix representation of the environment, with $\alpha$ the virtual indices and $\sigma$ the physical indices to be contracted. Next we perform a Cholesky decomposition for $E$ to get

$$E_{a | \alpha} = \sum_{\alpha} \langle \sigma | \psi\rangle \langle \psi | \sigma \rangle_{a | \alpha}$$

where $K$ is the number of composite indices $a \alpha$. Thus we have, in matrix form, $M^{-1}EM^{-1} = 1$ (figure 5(a)). This implies that the basis set $\{|k\rangle\}$ defined by

$$\langle \sigma | k \rangle = \sum_{a | \alpha} \langle \sigma | \psi\rangle \langle \psi | \sigma \rangle_{a | \alpha}$$

forms an orthonormal basis set. At last, we insert $MM^{-1}$ into the original MPS between the environment and system blocks, and trace out the environment re-expressed in the basis $\{|k\rangle\}$. This is equivalent to getting rid of

![Figure 5](image-url)
the upper part above the slash in figure 5(a), leaving a tensor coefficient $M_{i,j,a,b}$. In this way we get the MPS representation of a mixed state in the system block. Notice that in the Cholesky decomposition, the number $K^*$ of non-zero $M$ is bounded by $K^* < \min(d^{n_{E}}, d)$ where $n_{E}$ is the number of sites in the environment block and $d$ is the dimension of the single-site Hilbert space. Rank deficiency (or $K^* < d$) occurs if $d^{n_{E}} < d$, making $M^{-1}$ ill-defined. However, we find this is harmless since $M^{-1}$ does not appear in the final representation. In practice, we use eigenvalue decomposition instead to get around the possible difficulty in the Cholesky decomposition. Finally, the overlap matrices $O_{L,E}(\psi^i, \psi^f)$ can be obtained by contracting the physical indices between two mixed states, see figure 5(b) for an illustration.

We remark that the labelling of sites in fermionic systems matters because the parity of electrons in the environment blocks trespassed by the system block may cause a negative sign. To avoid such a fermion sign problem, we always label the system blocks first, and the environment second. Notice that fermion signs are respected rigorously within the system and environment, respectively.

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