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Topological phases of one-dimensional fermions: An entanglement point of view

Ari M. Turner

Department of Physics, University of California, Berkeley, California 94720, USA

Frank Pollmann

Department of Physics, University of California, Berkeley, California 94720, USA and Institute of Physics, Academia Sinica, Taipei 11529, Taiwan

Erez Berg

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA (Received 29 August 2010; published 8 February 2011)

The effect of interactions on topological insulators and superconductors remains, to a large extent, an open problem. Here, we describe a framework for classifying phases of one-dimensional interacting fermions, focusing on spinless fermions with time-reversal symmetry and particle number parity conservation, using concepts of entanglement. In agreement with an example presented by L. Fidkowski and A. Kitaev [Phys. Rev. B **81**, 134509 (2010)], we find that in the presence of interactions there are only eight distinct phases which obey a \mathbb{Z}_8 group structure. This is in contrast to the \mathbb{Z} classification in the noninteracting case. Each of these eight phases is characterized by a unique set of bulk invariants, related to the transformation laws of its entanglement (Schmidt) eigenstates under symmetry operations, and has a characteristic degeneracy of its entanglement levels. If translational symmetry is present, the number of distinct phases increases to 16.

DOI: 10.1103/PhysRevB.83.075102

PACS number(s): 71.10.Pm, 64.70.Tg, 03.67.-a, 74.20.Rp

I. INTRODUCTION

Topological phases of matter are not characterized by a broken symmetry but rather by an underlying topological structure that distinguishes them from other, topologically trivial, phases. Such phases have attracted a great deal of attention recently, especially since the theoretical prediction 1-4and subsequent experimental observation^{5,6} of both twoand three-dimensional realizations of time-reversal invariant topological insulators. These (as well as their predecessor, the integer quantum Hall effect) can be thought of as band insulators characterized by the topological structure of their Bloch bands. Similarly, topological superconductors^{7–9} are characterized by the topological nature of their fermionic quasiparticle spectrum. All these systems can be understood from a noninteracting point of view. A complete classification of all topological phases of noninteracting fermions, given their symmetries, has been given in Refs. 8–10.

In the presence of electron-electron interactions, the Hamiltonian cannot be reduced to a single particle matrix. Therefore, strictly speaking, the above classification scheme of topological phases cannot be used. Nevertheless, in some classes of topological insulators, the topological order has been argued to be robust even in the presence of interactions by generalizing the corresponding topological invariant to the many-body case.^{10–12} In other classes, however, the situation in the interacting case remains unclear.

In a recent breakthrough, Fidkowski and Kitaev studied a one-dimensional model of spinless superconductors with time-reversal symmetry.¹³ They found that in the presence of interactions, the free-fermion classification breaks down from \mathbb{Z} to \mathbb{Z}_8 , i.e., there are only eight distinct phases that survive in the presence of interactions (as opposed to an infinite number without interactions). To the best of our knowledge, this is the first case where the noninteracting picture in a class of topological phases is found to be radically modified by interactions. Reference 13 constructs an explicit path in Hamiltonian space through which phases with different \mathbb{Z} numbers mod(8) can be connected and also discusses the stability of the edge states. However, a more general understanding of the classification of distinct phases in the presence of interactions (in particular, in terms of *bulk* properties of the ground-state wave function) is left open.

In this article, we develop a framework for classifying phases of interacting fermions in one dimension based on bipartite entanglement of the ground-state wave function. The fact that entanglement is a useful quantity to probe topological properties of wave functions has been shown in several recent publications; see, for example, Refs. 14-17. Our technique is based on a method which was introduced in Ref. 18 for classifying phases in spin systems. This method has also been developed more fully and shown to give a complete 1D classification by Ref. 19 (at least when translational symmetry is not required). Here we generalize the method to fermionic systems. We find that the eight phases found in Ref. 13 are indeed topologically distinct and characterize them in terms of a set of invariants. These phases cannot be continuously connected by adding any kind of interaction as long as time-reversal symmetry and fermion parity conservation are preserved.

The basic idea is to examine the behavior of the entanglement (Schmidt) eigenstates of a segment in the bulk of the system under the symmetry group of the system. Topologically nontrivial phases can be recognized by the presence of "fractionalized" modes in the entanglement spectrum, which transform differently under the symmetry group from the constituent microscopic degrees of freedom of the system (analogous to the half-integer spins at the ends of the spin one Heisenberg chain). The character of the entanglement spectrum cannot change without a bulk phase transition, at which the nature of the ground state changes abruptly or the correlation length diverges.

The behavior of the entanglement modes reflects the character of the *physical* topologically protected modes at the boundary of the system. However, unlike the edge modes, the entanglement spectrum represent a truly *bulk* property of the ground-state wave function, and as such, it is not sensitive to symmetry-breaking perturbations at the surface.

We start in Sec. II by introducing fermionic Hamiltonians with pairing terms through the example of a single Majorana chain model. The general framework to classify topological phases based on symmetry properties of the entanglement eigenstates is presented in Sec. III. We apply it to fermionic systems with time-reversal invariance and fermion number parity conservation and derive the invariants characterizing the eight distinct phases and the degeneracies in their entanglement spectrum. These phases are shown in the next section to have a \mathbb{Z}_8 group structure, defined through the rules for combining phases with different invariants. In Sec. IV, we demonstrate how to construct each phase by combining single chains. In Sec. V, we discuss the additional phases which arise if translational symmetry is imposed. The results are summarized and discussed in Sec. VI.

II. FERMIONIC MODELS WITH PAIRING TERMS

We will investigate time-reversal invariant one-dimensional systems of spinless fermions, in which the particle number is conserved modulo 2. (The classification of topological phases is most interesting in this case.) Such a situation can be realized in a system in contact with a superconductor. As a simple example, consider the following Hamiltonian²⁰:

$$H_0 = -\frac{t}{2} \sum_j (c_j^{\dagger} c_{j+1}^{\dagger} + c_j^{\dagger} c_{j+1} + \text{H.c.}) + u \sum_j c_j^{\dagger} c_j, \quad (1)$$

with $t, u \ge 0$. The operators $c_j^{\dagger}(c_j)$ create (annihilate) a spinless fermion on site *j*. The first term comprises hopping of fermions as well as the creation and annihilation of pairs of fermions while the second term acts as a chemical potential. The fermion parity operator

$$Q = e^{i\pi\sum_j n_j}$$

with $n_j = c_j^{\dagger} c_j$ commutes with H_0 as the total number of fermions N_{total} modulo 2 is conserved. Furthermore, the Hamiltonian is time-reversal symmetric. (For spinless fermions, time reversal is represented by complex conjugation.)

Let us begin by considering only the conservation of the fermion number parity. This symmetry of H_0 allows us to distinguish two different phases. The system undergoes phase transitions at t = u, but *no* local order parameter can be used to distinguish the two phases on either side of the transition. However, they can be distinguished by their edge states. In the phase u > t, the ground state for an open chain is unique while it is twofold degenerate for t > u.²⁰ If u = 0, one can check that these states are given by the equal weighted superposition of all configurations with fixed fermion parity (i.e., an even number or an odd number of particles). The

ground-state degeneracy in this case can be understood in term of degrees of freedom at the two ends. The two ground states cannot be distinguished by any local observable in the bulk, because in any finite region of either state, the parity can be either even or odd. However, the two states are distinguishable when the opposite ends are compared to one another: $c_N^{\dagger} c_1 + c_N^{\dagger} c_1^{\dagger} + \text{H.c.}$ has a different eigenvalue for the two states. Furthermore, we can transform the two ground states into each other by acting with either $c_1 + c_1^{\dagger}$ or $c_N - c_N^{\dagger}$ on the two ends of the chain. In other words, there is a single fermionic state that is split between the ends of the chain, and the observable described above measures its occupation number. The two states are degenerate because the only distinction between them is long range, while energy measures only local correlations. In the phase t < u, however, there is no such degeneracy. This picture remains true even if we include interactions as the arguments can be stated in a way that only requires the Hamiltonian to conserve the fermion parity, as explained in the next section.

The edge properties have a simple explanation in a different representation defined by the following transformation:

$$a_j = c_j + c_j^{\dagger} \tag{2}$$

$$b_j = -i(c_j - c_j^{\dagger}). \tag{3}$$

 a_j and b_j are Majorana operators; they obey the relations $\{a_i, a_j\} = \{b_i, b_j\} = \delta_{ij}, \ \{a_i, b_j\} = 0, \ a_i^{\dagger} = a_i, \ \text{and} \ b_i^{\dagger} = b_i.$ The fermion parity, $1 - 2n_j$ of a site, is given by ib_ja_j . Using these operators, H_0 can be written (up to a constant) as

$$H_{0} = \frac{i}{2} \left(t \sum_{j} b_{j} a_{j+1} + u \sum_{j} a_{j} b_{j} \right).$$
(4)

Observe that each unit cell now contains two operators. In the case where t = 0, u = 1, the ground state is described by $ia_jb_j = -1$, i.e., each site is vacant. In terms of these variables, the phase t = 1, u = 0, is also simple: $ib_ja_{j+1} =$ -1. (This can be regarded as the parity of a fermion shared between sites j and j + 1.) This requirement does not completely determine the ground-state wave function in an open chain, though, because it leaves a_1 and b_N free. There are therefore two degenerate states characterized by the occupation of the fermion shared between the ends, ib_Na_1 .

The presence of time-reversal symmetry leads to additional distinctions between phases. Quadratic, time-reversal invariant fermionic Hamiltonians with conservation of the fermion number mod(2) have been shown^{8,9} to support phases classified by an integer $n \in \mathbb{Z}$ (class BDI, according to Ref. 8). Each phase is characterized by having *n* gapless Majorana modes at each edge, and the different phases cannot be smoothly connected to each other without closing the bulk gap. It was later found¹³ that in the presence of interactions this classification breaks down to \mathbb{Z}_8 . Now we will begin the main discussion, whose goal is to show how the eight distinct phases in the general (interacting) case can be understood and classified according to properties of their entanglement eigenstates under the symmetries of the

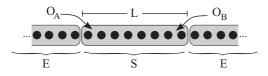


FIG. 1. Illustration of a bipartition of a 1D chain into a segment (S) of length L and a surrounding environment (E). The operators \mathcal{O}_A and \mathcal{O}_B act on the edges of the segment.

system, namely time reversal and fermion number parity conservation.

III. CLASSIFYING PHASES BY SYMMETRY PROPERTIES OF THE ENTANGLEMENT EIGENSTATES

In the preceding section, we discussed physical edge properties to characterize different phases. Below, we present an alternative method of classifying the phases, which *involves only the bulk*. This is achieved by examining the "entanglement spectrum"^{16,18,21–23} of a finite (but arbitrarily large) segment,^{14,15} embedded in an infinite system. The transformation law of the entanglement (or Schmidt) states under the symmetry group of the system can be used to distinguish between different phases, as we describe below.

We consider a bipartition of a 1D chain with periodic boundary conditions into a segment (S) of length L and a surrounding environment (E) of length $N \gg L$ as shown in Fig. 1. For the segment S, the reduced density matrix of the ground-state wave function $|\psi\rangle$ is given by

$$\rho_S = \operatorname{tr}_{\mathrm{E}}(|\psi\rangle\langle\psi|). \tag{5}$$

It is convenient to define an "entanglement Hamiltonian" \mathcal{H}_S such that

$$\rho_S = e^{-\mathcal{H}_S}.\tag{6}$$

Then, the low-"energy" states of \mathcal{H}_S are the most likely states of the segment *S* when the entire system is in its ground state. We call the eigenstates $|\phi_{\gamma}\rangle_S$ of \mathcal{H}_S "entanglement eigenstates" and the eigenvalues E_{γ} "entanglement eigenvalues." (These are the same as the Schmidt states defined by $|\psi\rangle = \sum e^{-\frac{E_{\gamma}}{2}} |\phi_{\gamma}\rangle_S |\chi_{\gamma}\rangle_E$, where $|\chi_{\gamma}\rangle_E$ are the corresponding Schmidt states of the environment.)

Our approach is based on an important observation for the entanglement Hamiltonian \mathcal{H}_S : The low "entanglement energy" excitations of \mathcal{H}_S in a *d*-dimensional system may be well described by a (d - 1)-dimensional effective Hamiltonian (see also Ref. 24 for an interesting discussion of this concept). We consider the entanglement spectrum of a sufficiently large one-dimensional segment *S* and focus on the "low-lying" entanglement states with $E_{\gamma} < E_{\text{cut}}$ (where E_{cut} is an arbitrary constant).

We now make a crucial observation: in a gapped system with a finite correlation length ξ ,²⁵ these states can be distinguished from each other only by their behavior within a certain distance of the ends of the segment *S*. This is justified by the following argument: suppose that we measure a correlation function $C(\ell) = \langle \mathcal{O}_E \mathcal{O}_S \rangle_{\psi}$, where \mathcal{O}_E acts on sites in the environment E and \mathcal{O}_S acts on sites in the segment (far away from the edges), respectively. ℓ is the minimal distance between the sites on which \mathcal{O}_E and \mathcal{O}_S act. We expect that as ℓ becomes large, $C(\ell) \to \langle \mathcal{O}_E \rangle_{\psi} \langle \mathcal{O}_S \rangle_{\psi}$. Let us take for \mathcal{O}_E an operator that projects onto a particular Schmidt state of the environment, say $|\chi_{\gamma}\rangle_{E}$. (\mathcal{O}_{S} can be any operator as long as it acts far from the edges of S.) When applied to the ground state, \mathcal{O}_E projects (through the entanglement between E and S) also onto the corresponding entanglement eigenstate $|\phi_{\gamma}\rangle_{S}$ of S. Thus, we have $\langle \mathcal{O}_S \rangle_{\phi_{\gamma}} \approx \langle \mathcal{O}_S \rangle_{\psi}$. That is, $\langle \mathcal{O}_S \rangle$ in each eigenstate of \mathcal{H}_S is the same as in the ground state; i.e., far enough from the edge of S, any eigenstate of \mathcal{H}_S behaves essentially like the ground state. Therefore, an operator acting far from the edge of S cannot distinguish different Schmidt states; its expectation value must be the same in all of them. (A simple generalization of the above argument, using an off-diagonal \mathcal{O}_E , shows that \mathcal{O}_S cannot connect different low-energy entanglement eigenstates if it is sufficiently far from the boundary.)

Furthermore, one can show (see Appendix A for the case of bosons) that any linear transformation applied to the subspace of low-entanglement energy eigenstates of S can be represented by a local operator acting on sites within a distance ℓ from either boundary of S with an accuracy that improves exponentially with ℓ . In particular, every symmetry operation of the system is a unitary operation acting on the entanglement eigenstates²⁶ and thus can be represented (within the low-entanglement basis) as a product of two operators \mathcal{O}_A , \mathcal{O}_B (Fig. 1), acting on sites near the left and right edges of S, respectively. (Note that \mathcal{O}_A , \mathcal{O}_B are specific for a particular ground state $|\psi\rangle$.) Thus, \mathcal{O}_A and \mathcal{O}_B form a (projective) representation of the symmetry group. Classifying the representations formed by \mathcal{O}_A , \mathcal{O}_B distinguishes different phases, which cannot be adiabatically connected unless a phase boundary is crossed. At the phase boundary, either the character of the ground state changes discontinuously or else the correlation length diverges and the two ends are no longer independent.

Let us demonstrate these principles through the case of an SO(3)-symmetric integer spin chain. If the segment S is sufficiently long, there can be situations in which entanglement states come in degenerate sets.¹⁸ This can be seen from the fact that, according to the argument above, any SO(3) rotation can be represented accurately (within the low-entanglement energy subspace) in terms of two generators, S_A and S_B , which act only within a distance ℓ of the left and right edges of S, respectively. Within this subspace, $S_{tot} \sim S_A + S_B$, where S_{tot} is the total spin. Both S_A , S_B can be block diagonalized into irreducible representations of SO(3) with well-defined angular momenta. Now, since \mathbf{S}_{tot} is an integer spin, there are two possibilities: either all the blocks in S_A and S_B form integer representations, or they all form half-integer representations. This distinguishes two phases: a "trivial" phase, in which S_A , S_B are both integers (e.g., a fully dimerized chain), and a "nontrivial" phase, in which they are half-integers (such as the Haldane phase of the spin-one chain²⁷). In the latter phase, all the entanglement energies of S must have a degeneracy of at least 4^{18} due to the even degeneracy at each end, guaranteed by the presence of the half-integer spin operators S_A and S_B . This is an alternative explanation of the symmetry protection of the Haldane phase, discussed in Refs. 18,28–31.

A. Fermion parity

We now turn to discuss fermionic systems. Let us consider a Hamiltonian H that conserves the fermion parity Q as defined in (2) with $Q^2 = 1$. We show that one can distinguish two phases, a "trivial" phase and a "nontrivial" one. In the "nontrivial" phase, a segment's entanglement spectrum is doubly degenerate. The double degeneracy is related to a single fermionic degree of freedom, which is split between the opposite ends of the segment.

Any eigenstate of H, and in particular the ground state $|\psi\rangle$, is also an eigenstate of Q. Hence the resulting reduced density matrix ρ_S and the entanglement Hamiltonian \mathcal{H}_S both commute with Q. The eigenstates $|\phi_{\gamma}\rangle$ of \mathcal{H}_S may therefore be classified by their Q eigenvalues ($q^S = +1$ if the fermion number N_F is even and $q^S = -1$ if N_F is odd.)

We now posit that it is possible to find an effective expression for Q within the low-entanglement energy subspace, of the form $Q \propto Q^A Q^B$, where Q^A and Q^B are local operators which act near the left and right edges of S, respectively. This is analogous to the example of spin described in the previous section, in which the total spin can be represented as a sum of operators acting on the left and right edges. [In the fermionic case, the decoupling of Q is multiplicative, since Q is itself a unitary symmetry rather than an SO(3) generator.]

Now, Q^A and Q^B can have interesting relationships: Q^A and Q^B may be two fermionic operators (that is, each contains an odd number of creation or annihilation operators) or they may both be bosonic. Note that Q^A or Q^B cannot contain a sum of bosonic and fermionic terms, because $Q \propto Q^A Q^B$ is bosonic.³²

If Q^A , Q^B contain an odd number of fermionic operators, then $Q^A Q^B = -Q^B Q^A$. To indicate when this "statistical correlation" between the two ends is present, define an angle $\mu = 0$ or π , so

$$Q^A Q^B = e^{i\mu} Q^B Q^A.$$
⁽⁷⁾

For $\mu = 0$ (π), $Q = Q^A Q^B$ ($-i Q^A Q^B$). The factor of *i* must be introduced in the latter case for consistency with the anticommutation of Q^A and Q^B , given that $Q^2 = (Q^A)^2 = (Q^B)^2 = 1$.

For example, consider the Hamiltonian in Eq. (1) with u = 0, t = 1. In this case, it is not difficult to show that there are only two entanglement eigenstates on the segment *S* (with a nonzero weight in the density matrix), the same two states as the ground states of the original Hamiltonian restricted to this segment. The fermion parity of these states is given by

$$Q = -i Q^A Q^B, (8)$$

where

$$Q^{A} = c_{1} + c_{1}^{\dagger}$$

$$Q^{B} = -i(c_{L} - c_{I}^{\dagger}).$$
(9)

We see immediately that Q^A and Q^B anticommute and therefore $\mu = \pi$. Furthermore, $[\mathcal{H}_S, Q^A] = [\mathcal{H}_S, Q^B] = 0$, which is also true in general. For any system with $\mu = \pi$, the above commutation relations imply that all the eigenvalues of \mathcal{H}_S come in degenerate pairs. To see this, note that Q and \mathcal{H}_S can be diagonalized simultaneously. Then, if $\mathcal{H}_S |\phi_{\lambda}\rangle = E_{\lambda} |\phi_{\lambda}\rangle$ and $Q |\phi_{\lambda}\rangle = q_{\lambda} |\phi_{\lambda}\rangle$ (where $q_{\lambda} = \pm 1$), then the state $|\psi_{\lambda}\rangle =$ $Q^A |\phi_{\lambda}\rangle$ is such that $\mathcal{H}_S |\psi_{\lambda}\rangle = E_{\lambda} |\psi_{\lambda}\rangle$ and $Q |\psi_{\lambda}\rangle = -q_{\lambda} |\psi_{\lambda}\rangle$, i.e., $|\psi_{\lambda}\rangle$ is an independent eigenstate with eigenvalue E_{λ} . Indeed, for the Hamiltonian (1) with u = 0, we find a doubly degenerate entanglement level with $E = \log 2$. (All other entanglement levels in that system have $E = \infty$.)

Note that, unlike the Haldane chain example in Sec. III, the entanglement spectrum is twofold (rather than fourfold) degenerate. This is a consequence of the fact that the degeneracy is not associated with either Q^A or Q^B alone; it is related to the occupation of the fermionic level formed by combining $Q^A + i Q^B$, i.e., it is *shared* between the two edges.

In a bosonic system, the states of the entanglement eigenstates can be represented by $|\phi_{\gamma}\rangle = |\alpha\beta\rangle$. Here α,β describe the states of the left and right ends of the chain; that is, they enumerate the eigenvalues of certain low-"energy" combinations of observables that are functions of ℓ sites at the respective ends. This factorization is possible for fermionic chains with $\mu = 0$ as well. However, for chains with $\mu = \pi$, the extra q_s variable describing the twofold degeneracy cannot be written in terms of local observables belonging to either end (i.e., the fermionic degrees of freedom cannot be measured independently at the two ends of the segment). Therefore, the entanglement states should be labeled by three variables, $|\alpha\beta q_s\rangle$, with the fermion parity q_s of the entire chain represented explicitly.³³

In a noninteracting system, the entanglement Hamiltonian is also noninteracting.^{34,35} It can be represented in terms of entanglement modes. The only subtlety is that some of these modes may be Majorana modes, which satisfy $m^2 = 1$; $m^{\dagger} = m$. There are two topologically distinct phases, depending on whether there are an even or an odd number of Majorana modes at each end of the segment. The Q^A and Q^B operators defined above can be found explicitly. Given that the left edge has N_f low-energy fermionic entanglement modes, $f_{A,\alpha}$ ($\alpha = 1, \ldots, N_f$), and N_m Majorana modes, $m_{A,\beta}$ ($\beta = 1, \ldots, N_m$), Q^A is given by

$$Q^{A} = \left(\prod_{\alpha} (-1)^{f^{\dagger}_{A,\alpha} f_{A,\alpha}}\right) \left(\prod_{\beta} m_{A,\beta}\right)$$
(10)

and similarly for Q^B . Note that Q^A is a bosonic operator if N_m is even (corresponding to $\mu = 0$) and a Majorana operator if N_m is odd ($\mu = \pi$).

When interactions are included, only the "total parities" Q^A , Q^B are well defined. The separate modes f_α , m_β can "decay" into other combinations of modes, but their total is closely related to the symmetry Q, as we have just outlined.

B. Time-reversal symmetry

We shall now examine the consequences of time-reversal symmetry for the degeneracies of the entanglement energies. It turns out that the combination of time reversal and fermion parity conservation can have nontrivial effects.

1. Bosonic models

Let us introduce the approach by reiterating the results for a bosonic chain in the presence of time-reversal symmetry with $[\mathcal{H}_S, T] = 0$. The eigenstates $|\phi_{\gamma}\rangle$ can be represented by $|\phi_{\gamma}\rangle = |\alpha\beta\rangle$, where α, β enumerate the low-"energy" states associated with the two edges. Entanglement eigenstates which differ in their α (β) index can be connected by a local operator close to the left (right) edge, respectively. The transformation of the eigenstates of \mathcal{H}_S factors into parts referring to the two ends (see Appendix A).

It can therefore be represented as a product of two unitary transformations U^A, U^B acting on the ends of the segment so

$$T|\alpha,\beta\rangle = \sum_{\alpha',\beta'} U^{A}_{\alpha'\alpha} U^{B}_{\beta'\beta} |\alpha'\beta'\rangle$$
(11)

and $[U^A, U^B] = 0$. For a discussion of subtleties related to the antiunitarity of *T*, see Appendix **B**. Applying *T* to an eigenstate twice yields

$$T^{2}|\alpha\beta\rangle = \sum_{\alpha',\beta',\alpha'',\beta''} U^{A}_{\alpha''\alpha'} U^{B}_{\beta''\beta'} (U^{A})^{*}_{\alpha'\alpha} (U^{B})^{*}_{\beta'\beta} |\alpha''\beta''\rangle.$$
(12)

Using $T^2 = 1$ and that the two ends of the segment are independent, it follows that

$$U^{A}(U^{A})^{*} = U^{B}(U^{B})^{*} = \exp(i\kappa)\mathbb{1}, \quad \kappa = 0, \pi.$$
(13)

We can thus distinguish two different phases, corresponding to $\kappa = 0, \pi$. Let us now focus on the consequences for the entanglement spectrum. Assume that $|\phi_{\gamma}\rangle$ is an eigenstate of \mathcal{H}_S with eigenvalue E_{γ} ; then $U^A |\phi_{\gamma}\rangle$, $U^B |\phi_{\gamma}\rangle$, $U^A U^B |\phi_{\gamma}\rangle$ are also eigenstates with the same eigenvalue because \mathcal{H}_S commutes with U_A and U_B . If $\kappa = \pi$, the unitaries U^A, U^B are antisymmetric and thus the four states are mutually orthogonal, resulting in a fourfold degeneracy of the entanglement spectrum. If $\kappa = 0$, the entanglement spectrum does not necessarily have any degeneracies. For example, in the Haldane phase of spin-1 chains, we find $\kappa = \pi$ and therefore the entire entanglement spectrum of a segment *S* is fourfold degenerate.^{18,36}

This method may be generalized to give a classification of phases with any given set of symmetries. For each relationship between the physical symmetries (e.g., $T^2 = 1$ in the case just described), there is a corresponding relationship between the factored symmetries of the entanglement spectrum,¹⁸ in which certain phases (e.g., κ) can appear. Certain combinations of these phases are "gauge invariant" (independent of how the phases of the factored symmetries are chosen). These combinations distinguish between topological phases. In fermionic models, an additional possibility is that symmetry operators at opposite ends may either commute or anticommute, as described in the previous section.

2. Fermionic models

We now consider a Hamiltonian which has both fermion parity conservation with $Q^2 = 1$ and time-reversal symmetry with $T^2 = 1$. In the presence of both symmetries, we show that each of the two phases defined in the previous section ($\mu = 0, \pi$) can be subdivided into four different phases. Furthermore, we discuss the consequences for the entanglement spectrum in each case. As T simply takes the complex conjugate (spin degrees of freedom are not considered here), it does not change the total fermion number and thus [T,Q] = 0. We will now classify the phases by examining how the properties of the factored versions of Q and T depart from the relations of the full transformations, $T^2 = 1$, [T,Q] = 0.

We first consider the case $\mu = 0$, i.e., $[Q^A, Q^B] = 0$. Then, both Q^A and Q^B are bosonic operators and can be diagonalized simultaneously. Then, we distinguish two cases: $Q^A T = e^{i\phi}TQ^A$ with $\phi = 0,\pi$, and similarly for Q^B . Note that ϕ has to be the same for Q^A and Q^B , since $Q = Q^A Q^B$ satisfies [T, Q] = 0. If $\phi = \pi$, time reversal changes the parity of the fermion number in either end. (A similar situation occurs at the vortex cores of time-reversal invariant topological superconductors.³⁷) We now examine the two cases $\phi = 0,\pi$ separately, showing how to define a third angle κ in each case.

 $(\mu = 0, \phi = 0, \kappa = 0 \text{ or } \pi)$: The case $\phi = 0$ is analogous to the bosonic case considered above, with two phases, one corresponding to $\kappa = \pi$, characterized by a fourfold degenerate entanglement spectrum of a segment, and one to $\kappa = 0$, in which there is no necessary degeneracy in the entanglement spectrum.

 $(\mu = 0, \phi = \pi, \kappa = 0 \text{ or } \pi)$: If $\phi = \pi, U^A$ and U^B (defined through $T = U^A U^B$; see Appendix B for a precise explanation of this factorization.) are both fermionic operators, since they change the fermion parity. We know that $T^2 = U^A U^B (U^A U^B)^* = -U^A U^{A*} U^B U^{B*} = 1$. This can be satisfied only if $U^A (U^A)^* = \exp(i\kappa) 1$ and $U^B (U^B)^* =$ $-\exp(i\kappa) 1$ with $\kappa = 0, \pi$. To understand the degeneracies, note that $\{Q^A, U^A\} = 0$ and $\{Q^B, U^B\} = 0$, where both U^A and U^B commute with \mathcal{H}_S . $\{\cdot, \cdot\}$ denotes an anticommutator.) Therefore, each entanglement level is fourfold degenerate, where the degeneracy corresponds to states with all possible combinations of $Q^A = \pm 1$ and $Q^B = \pm 1$.

Next, we consider the case $\mu = \pi$. In this case, $\{Q^A, Q^B\} = 0$, so these two operators cannot be diagonalized simultaneously. Rather, every entanglement eigenstate can be labeled by the eigenvalue $q = \pm 1$ of the parity operator $Q = -iQ^AQ^B$, where $|\alpha\beta,q=\pm1\rangle$ are degenerate. Since [T,Q] = 0, we must have either $[T,Q^A] = 0$ and $\{T,Q^B\} = 0$ or vice versa. Therefore, we define a parameter $\phi = 0,\pi$ such that $TQ^A = e^{i\phi}Q^AT$ and $TQ^B = e^{i(\phi+\pi)}Q^BT$.

In this case ($\mu = \pi$), phases with $\phi = 0$ and π behave very similarly. To see this, we just note that if $\phi = \pi$ then QTcommutes with Q^A . Therefore, we will define a modification of time reversal that commutes with Q^A , T' := QT if $\phi = \pi$ and T' := T if $\phi = 0$. Let the factors of T' be $T' = U^{A'}U^{B'}$. One can check that $U^{A'}, U^{B'}$ are bosonic. The entanglement spectrum can be divided into two sectors with a fixed value of q. The operator $U^{A'}$, being bosonic, depends only on α,β and hence acts the same way on both sectors. Define κ by $e^{i\kappa} \mathbf{1} = U^{A'}U^{A'*} = U^{B'}U^{B'*}$. The possible values for κ are 0 and π .

 $(\mu = \pi, \phi = 0 \text{ or } \pi, \kappa = 0)$: If $\kappa = 0$, each entanglement eigenstate in each q sector can be singly degenerate. Therefore, counting the $q = \pm 1$ degeneracy, each entanglement eigenstate has a minimal degeneracy of 2.

 $(\mu = \pi, \phi = 0 \text{ or } \pi, \kappa = \pi)$: If $\kappa = \pi$, the spectrum in each of the $\pm q$ sectors is fourfold degenerate (for the same

TABLE I. Degeneracies and addition table. All possible phases of fermions are realized by simply taking copies of some number of Majorana chains (see next section); the first column is the number of chains. The next column gives the parameters classifying a given state. The third column gives the degeneracy of the Schmidt spectrum, counting *both* ends.

Number of chains	(μ,ϕ,κ)	Degeneracy of segment
1	$(\pi, 0, 0)$	2
2	$(0, \pi, \pi)$	4
3	(π,π,π)	8
4	$(0,0,\pi)$	4
5	$(\pi, 0, \pi)$	8
6	$(0, \pi, 0)$	4
7	$(\pi,\pi,0)$	2
8	(0,0,0)	1

reasons as in the bosonic case above with $\kappa = \pi$, i.e., there is a Kramer's doublet at each edge). Taking the $q = \pm 1$ degeneracy into account, every entanglement eigenstate is at least eightfold degenerate.

There are therefore eight different phases classified by triplets (μ, ϕ, κ) , where each entry is 0 or π . $\mu = \pi$ if there are Majorana modes at the ends of the segment, $\phi = \pi$ if time reversal and Q^A anticommute, and $\kappa = \pi$ if $U^A(U^A)^* = -1$ (leading to Kramers' doublets at the edges of the segment). Since, as long as the time reversal and fermion parity symmetries are preserved, (μ, ϕ, κ) can take only the values 0 or π , and they cannot change smoothly; the only way for them to change is through a nonanalytic change of the ground-state wave function, i.e., a quantum phase transition.

The eight different phases and their corresponding minimal degeneracies are summarized in Table I. The degeneracies illustrate a distinction between interacting and noninteracting systems. As we will show in Sec. IV, the eight distinct phases can be realized by taking M copies of a single chain in the large t phase, where M = 1, ..., 8. Without interactions, the degeneracy of the Schmidt spectrum would be equal to 2^M . Interactions can partly lift this degeneracy but cannot connect the eight phases defined by (μ, ϕ, κ) adiabatically.

IV. ADDITION OF PHASES

The eight phases we have just obtained obey a group structure, which is defined by the rules of "adding" them together. This group turns out to be \mathbb{Z}_8 . The addition rules reveal interesting distinctions between bosons and fermions. We will work out the addition table in some detail.

Two systems can be added together by placing them side by side: hence if one system is in phase P_1 and another is in P_2 , then the combined "ladder" system is in phase $P_1 + P_2$. (The combined system then remains in $P_1 + P_2$ even when the two constituent systems are coupled, as long as the coupling Hamiltonian is symmetric under time-reversal and fermion parity, and the bulk gap does not collapse.) This rule creates a finite group for a given set of symmetries. In particular, every element in this group has an inverse and the trivial phase is the identity element. The distinction between fermionic and bosonic systems is related to the inverse operation. If the system consists only of bosons, then the inverse element of any phase P is its complex conjugate (i.e., its time reversal):

$$P + P^* =$$
trivial phase. (14)

For an example, consider a spin one Heisenberg chain. A single chain cannot be adiabatically connected to the trivial phase because its ends transform as spin 1/2 degrees of freedom. However, as shown in Ref. 38, two coupled chains can be connected continuously to the rung singlet phase (i.e., a product state of spin zeros on the rungs). The two chains are no longer distinguished from the trivial phase by their ends because the two half-integer spins couple to form integer spin states.

In general, phases of bosonic chains are distinguished by the projective representation of the symmetry groups acting on the entanglement eigenstates (see Ref. 18). Each element in the symmetry group \sum is represented in the entanglement eigenbasis as a left-hand unitary matrix $U^A(\Sigma)$ acting on the left index of the state and a right-hand matrix $U^B(\Sigma)$ acting on the right index. Then the combined operation of two elements Σ_1 and Σ_2 is represented by $U^A(\Sigma_1 \Sigma_2) = e^{i\rho_A(\Sigma_1, \Sigma_2)}U^A(\Sigma_1)U^A(\Sigma_2)$, and similarly for U^B . To see that $P + P^*$ is trivial, consider the eigenstates of the entanglement Hamiltonian for a segment in the combined system

$$|\alpha\beta\rangle_{\text{coupled}} = |\alpha_1\beta_1\rangle_P |\alpha_2\beta_2\rangle_{P^*}.$$
 (15)

The left-hand matrix U^A representing a symmetry Σ for the coupled system is

$$U^{A,\text{coupled}}_{\alpha'_1\alpha'_2;\alpha_1\alpha_2}(\Sigma) = U^{A}_{\alpha'_1\alpha_1}(\Sigma)U^{A*}_{\alpha'_2\alpha_2}(\Sigma),$$
(16)

where the second factor is complex conjugated because the second chain is time reversed. Hence, the phase factors cancel, $U^{A,\text{coupled}}(\Sigma_1)U^{A,\text{coupled}}(\Sigma_2) = U^{A,\text{coupled}}(\Sigma_1\Sigma_2)$, and the resulting system is in a trivial phase.

Now we can try to build more complicated phases out of simpler ones by placing them side by side. For bosonic systems, this procedure does not generate new phases in the presence of time-reversal symmetry. Time-reversal symmetry and Eq. (14) imply that P + P = 0. Hence starting from one phase, it is not possible to get more than two phases (the original phase and the trivial phase). There may be additional phases that would have to be built up from independent starting points. The group is always a product of \mathbb{Z}_2 's, in other words.

However, for fermionic spin chains, P and P^* are not necessarily inverses. The *p*-wave superconducting state P_1 described by Eq. (1) with $t > \mu$ which is an order 8 phase, as discovered by Fidkowski and Kitaev,¹³ is an illustration. Equation (16) breaks down because operators on the two chains can anticommute with each other. In fact, starting from a single Majorana chain, we can generate all possible combinations of μ , ϕ , and κ . We now demonstrate this idea for a number of examples. We start with the Majorana chain and double it repeatedly until we return to the trivial phase.

(i) Consider the Majorana chain, the ground state of Eq. (1) with t > u which is in the $(\mu, \phi, \kappa) = (\pi, 0, 0)$ phase. When two copies are combined together, the resulting phase has $(\mu, \phi, \kappa)_{\text{coupled}} = (0, \pi, \pi)$, i.e., the ends are not

Majorana fermions any longer, but time reversal changes the fermion parity of the ends. The fermion parity for the segment of the combined chain is given by $Q = Q_1 Q_2 =$ $(i Q_1^A Q_1^B)(i Q_2^A Q_2^B) = (Q_1^A Q_2^A)(Q_1^B Q_2^B)$, where the Q_n^A, Q_n^B are fermionic parity operators of a chain *n* with Majorana ends (see Sec. III A). One can measure the parities of the ends separately because $Q^A = -i Q_1^A Q_2^A$ and a similar operator on *B* are bosonic operators, so $\mu_{coupled} = 0$. On the other hand, $\phi_{coupled} = \pi$ because *T* anticommutes with Q^A on account of the factor of *i*. Furthermore, one finds that $\kappa_{coupled} = \pi$. (See Appendix B.)

(ii) Consider two chains with $(\mu, \phi, \kappa) = (0, \pi, \pi)$. Q_1^A, Q_2^A are bosonic, therefore $Q_{\text{coupled}}^A = Q_1^A Q_2^A$ is bosonic as well, and $\mu_{\text{coupled}} = 0$. Time reversal acting on the left edge is represented as $U_{\text{coupled}}^A = U_1^A U_2^A$. It anticommutes with Q_1^A , Q_2^A but commutes with their product, therefore $\phi_{\text{coupled}} = 0$. Since both U_1^A, U_2^A change the fermion parity, they both have to be *fermionic*. Therefore $\{U_1^A, U_2^A\} = 0$ and we get that

$$U_{\text{coupled}}^{A}U_{\text{coupled}}^{A*} = (U_{1}^{A}U_{2}^{A})(U_{1}^{A}U_{2}^{A})^{*}$$
$$= -U_{1}^{A}U_{1}^{A*}U_{2}^{A}U_{2}^{A*}$$
$$= -\mathbb{1}.$$
(17)

Hence $\kappa_{\text{coupled}} = \pi$, and the resulting phase is labeled by $(0,0,\pi)$.

(iii) Combining two chains with $(0,0,\pi)$ finally gives the trivial phase, because all the symmetries are represented by bosonic operators, therefore κ simply doubles to give 0 mod (2π) . This conforms with the fact that the Majorana chain is an order 8 element of the group.

Working out the addition rule in general gives the table of phases which are summarized in Table I. A concise way to describe the general addition rule is to define $\lambda \equiv \kappa + \phi \pmod{2\pi}$. Then we represent a state by a three-digit binary number $(\frac{\lambda}{\pi}, \frac{\phi}{\pi}, \frac{\mu}{\pi})$. These numbers add modulo 8 when the phases are combined.

V. TRANSLATIONAL INVARIANCE AND θ

If, in addition to fermion parity conservation, translational invariance is also present, the number of distinct phases is doubled. Below, we derive the associated invariant, θ , which can take the values 0 or π , independent of the invariants (μ, ϕ, κ) described above. The degeneracy of the entanglement spectrum, however, is not modified in either the $\theta = 0$ or π phases and is given by Table I.

Let us consider a fermionic chain with translational invariance. According to the Sec. III A, the fermion parity of a segment S = [1, L] extending from j = 1 to j = L (where L is much larger than the correlation length ξ) can be written as

$$Q(1,L) = e^{-i\frac{\mu}{2}} f(L) Q^{A}(1) Q^{B}(L).$$
(18)

Here, we have kept track explicitly of the position of the operators Q^A and Q^B and of an overall constant sign f(L) (which was absorbed into the definition of Q^A and Q^B before). Translational invariance removes the necessity of choosing the sign of Q^B (and Q^A) separately for each segment. This symmetry also allows us to write the parity operator of

the segment [1,L] in terms of those of the two segments $S_1 = [1,L']$ and $S_2 = [L'+1,L]$ (where $L', L - L' \gg \xi$) as

$$Q(1,L) = Q(1,L')Q(L'+1,L)$$

= $e^{-i\frac{\mu}{2}}f(L')f(L-L')$
 $\times Q^{A}(1)[e^{-i\frac{\mu}{2}}Q^{B}(L')Q^{A}(L'+1)]Q^{B}(L).$ (19)

Equating Eqs. (18) and (19) gives that, within the lowentanglement subspace, we must have

$$f(L')f(L-L')\left[e^{-i\frac{\mu}{2}}Q^B(L')Q^A(L'+1)\right] = f(L).$$
 (20)

Equation (20) can hold for every state in the lowentanglement subspace only if these states are all eigenstates of $e^{-i\frac{\mu}{2}}Q^B(L')Q^A(L'+1)$. The signs of Q^A and Q^B can be defined in such a way that the corresponding eigenvalue is 1. Then, we get that f(L')f(L - L') = f(L), which is solved by

$$f(L) = e^{i\theta L}.$$
 (21)

From the requirement that $[Q(1,L)]^2 = 1$, we get that θ can only take the values 0 or π . Thus, each of the eight phases found in the previous section is further split into two distinct phases, corresponding to the two allowed values of θ . For example, for the Majorana chain model [Eq. (1)], t = 0, u = +1 and t = 0, u = -1 describe distinct phases, although both have $\mu = 0$. The ground state has all sites occupied or unoccupied, corresponding to $\theta = \pi$ or $\theta = 0$, respectively.

Note that both θ and μ have a concrete consequence not only for the entanglement spectrum but also for the parity of the ground state in periodic chains. If the length of the chain is much larger than the correlation length, the parity depends only on μ and θ and the chain length, $(-1)^{(\mu+\theta L)/\pi}$. Thus, a phase with $\mu = \pi$ has an odd number of fermions on a chain of an even length.²⁰ The phase θ determines whether the parity of the ground state alternates as a function of *L*. This is shown in Appendix C.

VI. SUMMARY AND OUTLOOK

We have described a systematic procedure for classifying the phases of 1D interacting fermions. We focused on spinless fermions with time-reversal symmetry and particle number parity conservation. In the noninteracting case, these models are classified by an integer number, i.e., by \mathbb{Z} .^{8,9} We used concepts of entanglement to classify the phases in the presence of interactions. We derive an effective description of the dominant entanglement states which then allows us to recognize "topological" features based on projective representations of the symmetries. We found, in agreement with the results of Fidkowski and Kitaev (Ref. 13), that in the presence of interactions there are only eight distinct phases. Each of these eight phases is characterized by a unique set of bulk invariants (μ, ϕ, κ) , which can take the values 0 or π . These invariants are related to the transformation laws of the entanglement eigenstates under symmetry operations, and the phases have a characteristic degeneracy of entanglement levels. Furthermore, the phases obey a \mathbb{Z}_8 group structure and each of the eight phases can be generated by adding single chains together. All possible phases and the addition rules are summarized in Table I. If translational symmetry is also present, the number of distinct phases increases to 16.

The symmetries we have focused on describe only one of the 10 Altland-Zirnbauer classes³⁹ of topological insulators. The framework described here can also be used to show how the phases in the other classes are modified by interactions. To analyze each of the classes of topological insulators, one only has to determine the appropriate algebra of symmetries and then determine the possible projective representations of this algebra.

Interactions cause the meaning of the Altland-Zirnbauer classes to bifurcate, however. At the mean-field level, a superconductor has an emergent particle-hole symmetry in its band structure. Thus, the classes which have a particle-hole symmetry can be interpreted as describing either superconductors or systems that have a true particle-hole symmetry (such as the Hubbard model for fermions with spin on a bipartite lattice at half-filling). When interactions are included, these two interpretations are distinct. Thus, the class BDI, for example, has particle-hole and time-reversal symmetry. This can be interpreted as describing superconductors. This means that one symmetry, particle conservation, breaks down, and only fermion parity Q is left. The only two symmetries are T and Q, giving the problem treated here. BDI can be interpreted instead as describing systems with a true particle-hole symmetry Cthat reverses the sign of $\langle n_i \rangle - \bar{n}$. (Here, n_i is the occupation number of a site and \bar{n} is the mean occupation number.) In this case, particle number N is conserved, and besides this there are two other symmetries T and C. These satisfy the algebra $T^2 = C^2 = 1$, $CN + NC = 2\bar{n}L$, where L is the length of the system. (Every other pair of these symmetries commute.) The set of phases differs for the two interpretations; particle number conservation rules out Majorana fermions. A complete classification of systems in all Altland-Zirnbauer classes in one dimension, following either of the two interpretations of particle-hole symmetry mentioned above, would be an interesting project for future work.

A generalization of these results to higher-dimensional systems is an interesting (and challenging) open problem. In some of the symmetry classes of topological insulators and superconductors, strong arguments have been given that the noninteracting classification does not change when interactions are included. This is particularly clear when the topological invariant is related to a quantized physical response, e.g., in the integer quantum Hall effect^{11,12} and in 3D time-reversal invariant topological insulators.¹⁰ However, for other classes, the situation is less clear. For example, the noninteracting classification of 3D chiral superconductors is \mathbb{Z} ,^{8,9} similar to the one-dimensional case considered here. It would be interesting to consider the effect of interactions on the phase diagrams of such systems.

Note. As we were writing this article, we learned that a similar classification is being worked out by Fidkowski and Kitaev.⁴⁰ Our results are consistent with theirs.

ACKNOWLEDGMENTS

We thank Lukasz Fidkowski and Shinsei Ryu for useful discussions. E.B. was supported by the NSF under Grants No. DMR-0705472 and No. DMR-0757145. F.P. and A.M.T.

acknowledge support from ARO Grant No. W911NF-07-1-0576.

APPENDIX A: LOW-ENERGY OPERATORS AND THE ENDS OF THE CHAIN

An intuitive argument, given above, suggests that lowenergy operators acting on the entanglement eigenstates may be represented approximately by operators located near the ends of the chain: in each Schmidt state $|\alpha\beta\rangle_S$ the expectation values of the spin and other operators have some particular spatial dependence near the ends of the chain depending on α and β , but this decays exponentially to the ground state away from the ends. Therefore it should be possible to transform between these states by using operators defined on just the ends. A special case is the effective representations of symmetries in terms of operators at the ends of the segments, which we used to define the topological phases.

To see that these effective operators exist, one can use a matrix product state representation⁴¹ of the wave function. (We focus here just on bosonic systems. For systems including fermions a similar argument can be developed using bosonization but the discussion of this general result gets complicated in the $\mu = \pi$ phases.)

A basis for the low-energy operators can be constructed as follows. For each fixed choice of α_1 and α_2 let $\mathcal{O}^A(\alpha_2,\alpha_1)$ be the operator that transforms α_1 into α_2 .

We will now give an approximate representation for $\mathcal{O}^A(\alpha_1, \alpha_2)$ that gives the correct transformation of *low-energy* states of \mathcal{H}_S . Let the matrices Γ_m , Λ define the bulk state (*m* varies over a basis for the physical Hilbert space). The ground-state wave function of a ring of length *N* is given by

$$|\psi\rangle = \sum_{\{m_i\}} \operatorname{tr} \left(\Gamma_{m_1} \Lambda \Gamma_{m_2} \dots \Lambda \Gamma_{m_N} \Lambda \right) |m_1 m_2 \dots m_N \rangle, \quad (A1)$$

where Γ_m , Λ can be brought into a canonical form, satisfying $\sum_m \Gamma_m \Lambda \Gamma_m^{\dagger} = \sum_m \Gamma_m^{\dagger} \Lambda \Gamma_m = \mathbb{1}$, where Λ is a diagonal matrix with non-negative entries.^{42,43} For a generic wave function, Γ_m , Λ are infinite dimensional.

Let us define the states $|\alpha\beta\rangle_{1L}$ of a segment of the chain stretching from 1 to *L*, where L < N, as

$$|\alpha\beta\rangle_{1,L} = \sum_{\{m_i\}} \left(\Gamma_{m_1} \Lambda \Gamma_{m_2} \dots \Lambda \Gamma_{m_L} \right)_{\alpha\beta} |m_1 m_2 \dots m_L \rangle. \quad (A2)$$

When *L* is large these states are nearly orthonormal, that is $|\langle \alpha'\beta'|\alpha\beta\rangle_{1,L} - \delta_{\alpha'\alpha}\delta_{\beta'\beta}| \sim Ce^{-\frac{L}{\xi}}$, where ξ is the length scale for the decay and *C* is a constant depending on the indices. In this limit, $|\alpha\beta\rangle_{1L}$ are the entanglement eigenstates of the segment. On the other hand, if the length of the chain is fixed and $\alpha, \beta, \alpha', \beta'$ increase, the orthonormality must eventually break down for high enough $\alpha, \beta, \alpha', \beta'$ (since the Hilbert space of a segment of length *L* is finite while the dimension of the matrices is infinite for a typical wave function). Indeed, *C* grows as a function of $\alpha, \alpha', \beta, \beta'$.

The ground-state wave function (A1) can now be written as

$$|\psi\rangle = \sum_{\alpha,\beta} \lambda_{\alpha} \lambda_{\beta} |\alpha\beta\rangle_{1,L} |\alpha\beta\rangle_{L+1,N}.$$
 (A3)

This gives the Schmidt decomposition into states of the environment $|\alpha\beta\rangle_{L+1,N}$ and states of the chain $|\alpha\beta\rangle_{1,L}$, with a Schmidt eigenvalue $\lambda_{\alpha}\lambda_{\beta}$ [or, equivalently, an entanglement energy $E = E_{\alpha} + E_{\beta} = -2(\ln \lambda_{\alpha} + \ln \lambda_{\beta})$]. The Schmidt eigenstates become orthogonal to each other in the limit $N \to \infty$ and $L \to \infty$.

We can now give an "effective" expression for \mathcal{O}^A in terms of local operators acting on sites $1, \ldots, \ell$ (near the left edge of the segment [1,L]), valid for a low entanglement-energy subspace with $E_{\alpha} < E_{\text{cut}}$. E_{cut} is a cutoff which depends on ℓ . The accuracy of our effective expression improves as ℓ becomes larger (provided that $N \gg \ell$). Define

$$\mathcal{O}_{\alpha_{2}\alpha_{1}}^{A,\text{eff}} = \sum_{\gamma=1}^{\chi} |\alpha_{2}\gamma\rangle_{1,\ell} \langle \alpha_{1}\gamma|_{1,\ell}, \qquad (A4)$$

where χ is a cutoff of the entanglement spectrum that satisfies $E_{\gamma=1,...,\chi} < E_{\text{cut}}$. $\mathcal{O}_{\alpha_2\alpha_1}^{A,\text{eff}}$ acts only on the ℓ first sites of the segment [1,*L*].

We now apply $\mathcal{O}_{\alpha_2\alpha_1}^{A,\text{eff}}$ to the state Eq. (A2), with $\alpha \leq \chi$. This state can be expanded $\sum_{\gamma'} |\alpha\gamma'\rangle_{1\ell}\lambda_{\gamma'}|\gamma'\beta\rangle_{\ell+1,N}$. Using the approximate orthornormality of the states on the segment from 1 to ℓ , we find that the operator in fact transforms α_1 into α_2 . Intuitively, the sum over γ , the state of the internal end of the ℓ -site segment ensures that this operator keeps the right type of entanglement between the left and right side of the "cut" at ℓ . The error of (A4) scales as $F(\chi)e^{-\frac{\ell}{\xi}}$, where $F(\chi)$ is a function of χ . [$F(\chi)$ grows with χ , hence, to deal with a larger range of "energies," a larger value of ℓ must be used. This is because, as the "energy" of a state increases, it penetrates further into the bulk.]

Note that $\mathcal{O}_{\alpha_2\alpha_1}^{A,\text{eff}}$ does not transform high-entanglement energy states correctly, that is states such as $|\alpha\beta\rangle_{1N}$ with $\alpha > \chi$. This is because $|\alpha_1\gamma\rangle$ and $|\alpha\gamma'\rangle$ are orthonormal only if they are both low-energy states. This limitation is unavoidable: it is not possible to find a perfect representation for an operator, such as Q, in terms of just the ℓ sites near each end. One can add an extra particle somewhere outside of the reach of these sites, changing the value of Q but not of an observable on the ends of the chain. The *physical* energy of this state may not be much greater than the gap. However, not being able to describe states like this is not a problem when one is studying the ground state of the system: its *entanglement* energy is large, which means that it contributes negligibly to the value of any observable in the ground state.

APPENDIX B: FACTORING ANTIUNITARY OPERATORS

In the analysis of time-reversal symmetry, we defined a parameter κ by factoring T into two operators U^A and U^B , acting near the two opposite edges of the segment. To determine how chains add to one another, it is necessary to know the commutation and anticommutation properties of these operators. We ignored a small detail, however: since T is antiunitary, it cannot be factored either as the product of two unitary or two antiunitary operators. One solution is just to explicitly write how T transforms the basis states as we did in Eqs. (11) and (12). This becomes cumbersome after a while, however, and later in the text we have treated U^A and U^B as unitary operators in Hilbert space, without keeping explicit track of their indices. Here we will explain the meaning of this.

We will first discuss the bosonic case. Equation (11) gives the action of T only on basis states. Taking a superposition gives a factorization of T that is correct for any state:

$$T = U_A U_B K, \tag{B1}$$

where U_A and U_B are *unitary* operators at the two ends and *K* is defined by

$$K\sum_{\alpha\beta}a_{\alpha\beta}|\alpha\beta\rangle = \sum_{\alpha\beta}a_{\alpha\beta}^{*}|\alpha\beta\rangle, \tag{B2}$$

where $a_{\alpha\beta}$ are arbitrary coefficients. We can now define κ by $(U^A K)^2 = e^{i\kappa} \mathbb{1}$. Thus, $U^A K$ is an antiunitary symmetry squaring to $-\mathbb{1}$ in the nontrivial phase as in Kramers' theorem. Note that this equation is equivalent to the definition given above, Eq. (13). This is because $K U^A K^{-1} = U^{A*}$ when the matrices are represented in the basis $|\alpha\beta\rangle$. (Note that the complex conjugate of a matrix depends on the basis being used, unlike the adjoint.)

We can argue physically that operators U^A and U^B satisfying Eq. (B1) can always be found. Consider the ratio TK^{-1} between T, which is represented by complex conjugation in terms of the microscopic degrees of freedom, and K which describes complex conjugation in the entanglement eigenstate basis. This operator is unitary. Furthermore it acts independently on the two ends: one may check that $K\mathcal{O}^{A,B}K$ is an operator acting on end A or B respectively, by expressing it in the basis of entanglement eigenstates. Hence $TK^{-1}\mathcal{O}^{A,B}(TK^{-1})^{-1}$ also has this property.

The operator $U^A K$ used to define κ is nonlocal. It does not commute with operators at end *B*, because it takes complex conjugates of them. However, we can still argue that κ is well defined: Square Eq. (B1): $\mathbb{1} = U^A U^B K U^A U^B K$. Since $K^2 =$ $\mathbb{1}$, we can write this also as $\mathbb{1} = U^A U^B (K U^A K) (K U^B K)$. $K U^A K$ is an operator which acts on end *A*, therefore it commutes with U^B . Hence $\mathbb{1} = [U^A (K U^A K)][U^B (K U^B K)]$. Since the two factors are local, each must be a pure phase, hence $(U^A K)^2 = e^{i\kappa} \mathbb{1}$.

Now the operators U^A and U^B are not uniquely defined because *complex conjugation*, *K*, *is basis dependent*. Changing the basis of eigenstates in which Eq. (B2) is imposed (e.g., multiplying the entanglement states by phase factors) changes *K*. This does not change topological properties like the value of κ , however: the unitary transformation that changes the basis can be carried out continuously, starting from the identity. In this process, κ cannot change because it can only be 0 or π .

For fermionic systems with $\mu = 0$, one can decompose T using Eq. (B1). When $\mu = \pi$, the situation is more complicated because the parity eigenvalue q cannot be associated with either one of the edges. We have to make sure that K still maps operators at each end of the system to other operators at that end. In particular, $KQ^{A}K$ must be a local operator at end A.

This condition is satisfied if *K* is defined to be complex conjugation in the basis $|\alpha\beta q\rangle$ provided that Q^A and Q^B are represented by either purely real or purely imaginary matrices in that basis. One way to satisfy this requirement is to first choose a basis for q = +1 and then to construct the states in the sector from them, $|\alpha\beta, q = -1\rangle = Q^A |\alpha\beta, q = +1\rangle$. Then Q^A

is represented by σ^x , acting in the $q = \pm 1$ basis. In this basis, each state is an eigenstate of $Q = \sigma^z$. Last, $Q^B = iQQ^A = \sigma^y$. Since Q^A is real and Q^B is imaginary, the two ends are not mixed by applying K. (If the relative phases of the basis states are changed, then simple complex conjugation would mix Q^A and Q^B into one another.) We have implicitly taken the convention that Q^A is real and Q^B is imaginary throughout the paper.

Now let us show how to calculate κ when two $(\mu, \phi, \kappa) = (\pi, 0, 0)$ chains are combined. The factorization $T = U^A U^B K$ must be carried out in a basis of states of the form $|\alpha\beta\rangle$, according to our conventions. One basis for the states on the two chains together is given by $\{|\pm\rangle_1|\pm\rangle_2\}$ (where the sign represents the values of q_1, q_2 . (We do not explicitly write the bosonic indices α, β .) These states map to themselves under time reversal. However, U^A and U^B cannot be the identity because we know they must be fermionic; the error is that this is the wrong basis for defining K by simple complex conjugation.

We must transform the states to a basis in which there is no entanglement between the ends; we use states that are eigenvectors of the local operators $Q^A = -iQ_1^AQ_2^A$ and $Q^B = iQ_1^BQ_2^B$, namely $|q_Aq_B\rangle$. (The relative minus sign between Q^A and Q^B ensures that the total parity is $q_Aq_B = q_1q_2$.)

To construct the basis, first find an eigenfunction of Q^A and Q^B with eigenvalues +1, (choose the phase arbitrarily):

$$|+_{A}+_{B}\rangle = \frac{1}{\sqrt{2}}(|+\rangle_{1}|+\rangle_{2} - i|-\rangle_{1}|-\rangle_{2}).$$
 (B3)

Now generate the other basis states from this by applying Q_1^A and Q_1^B :

$$|-_{A}+_{B}\rangle := Q_{1}^{A}|+_{A}+_{B}\rangle = \frac{1}{\sqrt{2}}(|-\rangle_{1}|+\rangle_{2}-i|+\rangle_{1}|-\rangle_{2})$$

$$|+_{A}-_{B}\rangle := -iQ_{1}^{B}|+_{A}+_{B}\rangle = \frac{1}{\sqrt{2}}(|-\rangle_{1}|+\rangle_{2}+i|+\rangle_{1}|-\rangle_{2})$$

$$|-_{A}-_{B}\rangle := Q_{1}^{A}|+_{A}-_{B}\rangle = \frac{1}{\sqrt{2}}(|+\rangle_{1}|+\rangle_{2}+i|-\rangle_{1}|-\rangle_{2}).$$
(B4)

The phases are just conventions in the first two definitions, and the phase in the third equation follows from the independence of the ends: Q_1^A has to act on q_A the same way no matter what the value of q_B is. Now it is clear that T switches the fermion parity of each end in this basis, since changing the sign of *i* exchanges the states $|q_A q_B\rangle$ and $|-q_A, -q_B\rangle$.

Now we can define K to map each of *these* basis states to itself. Clearly, $T = Q_2$ because Q_2 exchanges the same pairs of wave functions as T or, more precisely, $T = Q_2 K$. Hence $U^A = -iQ^A$ and $U^B = Q^B$. One can check that $(U^A K)^2 = -1$, so $\kappa = \pi$.

Note that, in spite of all this trouble, the value of κ in a phase with $\mu = 0, \phi = \pi$ does not have any physical significance the fourfold degeneracy of the spectrum is already explained by the fact that $\phi = \pi$. The reason T changes fermion parity at the ends is that the two ends can only be disentangled by a change of basis that includes complex phases.

APPENDIX C: PARITY OF THE GROUND STATE ON A PERIODIC CHAIN

The parity of the ground state on a periodic chain is given by $e^{i(\theta L + \mu)}$. This follows from a fact in Sec. V: Consider two subsegments of the chain, one ending at X and the other starting at X + 1. The ground-state wave function is an eigenfunction of the following:

$$e^{-i\frac{\mu}{2}}Q^B(X)Q^A(X+1)|\psi\rangle = |\psi\rangle.$$
(C1)

When $\mu = \pi$, this relation describes the correlations between the Majorana degrees of freedom in adjacent segments of the chain.

We now suppose the periodic chain has length *L* and break it at two places, between *L'* and *L'* + 1 and between *L* and 1. The total fermion parity of the ground state is the product of the parity on the two segments, $[e^{i(\theta L' - \frac{\mu}{2})}Q^A(1)Q^B(L')][e^{i(\theta(L-L') - \frac{\mu}{2})}Q^A(L' + 1)Q^B(L)]$. Rearranging and using Eq. (C1), the ground-state parity comes out as $e^{i(\theta L + \mu)}$. The extra minus sign when $\mu = \pi$ comes from anticommuting the *Q* operators.

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- ³³In a chain with $\mu = \pi$, operators on both sides of the chain can change q_s . The distinction between operators acting on the left and those acting on the right end is that they are proportional to σ_x, σ_y respectively. Though these act on the same variable q_s , they anticommute.
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