Band Topology of Insulators via the Entanglement Spectrum

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How do we uniquely identify a quantum phase, given its ground state wave-function? This is a key question for many body theory especially when we consider phases like topological insulators, that share the same symmetry but differ at the level of topology. The entanglement spectrum has been proposed as a ground state property that captures characteristic edge excitations. Here we study the entanglement spectrum for topological band insulators. We first show that insulators with topological surface states will necessarily also have protected modes in the entanglement spectrum. Surprisingly, however, the converse is not true. Protected entanglement modes can also appear for insulators without physical surface states, in which case they capture a more elusive property. This is illustrated by considering insulators with only inversion symmetry. Inversion is shown to act in an unusual way, as an antiunitary operator, on the entanglement spectrum, leading to this protection. The entanglement degeneracies indicate a variety of different phases in inversion symmetric insulators, and these phases are argued to be robust to the introduction of interactions.

I. INTRODUCTION

According to the Landau paradigm, phases of matter are classified by their pattern of symmetry breaking. While this accounts well for a number of experimentally observed phenomena, several exceptions have also cropped up. These include the fractional quantum Hall states and models of gapped spin liquids, which are characterized by a topological order: for these phases, the ground state degeneracy depends on the spatial topology of the sample. Perhaps the simplest phases for which a topological distinction is present are present are topological insulators and superconductors, composed of noninteracting particles. Experimental manifestations include the integer quantum Hall effect, spin-orbit induced $Z_3$ topological insulators in two dimensions and three dimensions as well as superfluid $He^3 - B$. Here, although there is a unique ground state and no symmetry difference from the trivial state, the topological distinction can manifest itself in different ways. These include a quantized response function (such as the Hall effect), or protected surface states. Given the subtleties associated with identifying topological phases, a new tool in this respect would be welcome.

Recently, it has been shown that studying the entanglement spectrum is a promising direction to identifying topological phases. Given the ground state wavefunction, and a partition of the system into a left and right half, one can perform a Schmidt decomposition:

$$|G⟩ = \sum_\alpha \frac{1}{\sqrt{Z}} e^{-E_\alpha} |\alpha_L⟩|\alpha_R⟩$$

Measuring the right half of the system shows it to be in state $|\alpha R⟩$ (called a Schmidt state) with probability $e^{-E_\alpha}/Z$. The quantities $E_\alpha$ comprise the entanglement spectrum, and are somewhat like “energies,” characterizing how unlikely a given fluctuation is to occur. (Note that we use the superscript “e” when describing the entanglement.) The entropy associated with this probability distribution is the entanglement entropy, which captures the same features of a phase as ground state degeneracy (or topological order). However, the entire spectrum can be expected to contain more information, allowing one to capture a wider class of distinctions. Even though entanglement related quantities are hard to measure directly, they can be conceptually very useful in identifying phases.

It has been shown for fractional quantum Hall states that although their bulk is gapped, the entanglement spectrum contains information about the edge modes. Numerical studies reveal that the largest entanglement eigenvalues (smallest $E_\alpha$) mimic the low-energy spectrum of surface modes. A relationship of this type is very interesting because the entanglement spectrum can be calculated entirely from the ground state wave function. In contrast, the edge modes are excited states of the Hamiltonian in a sample with boundaries. In a classical system, one would not be able to look at the ground state and determine its dynamics. But a quantum mechanical system, even in its ground state, has some zero-point motion that can give one a sense of its excited state properties. A direct classification of phases from their ground state wavefunctions is highly desirable and could be applied to cases where a candidate ground state (such as a Gutzwiller projected state) is available.

Here we study the entanglement spectrum in the context of the simplest class of topological phases - noninteracting topological band insulators. We show that whenever topological surface states are present, the entanglement spectrum, as a function of the momentum parallel to the cut, also has protected entanglement modes. Essentially, the entanglement spectrum is known to result from diagonalizing an operator, and this operator can be viewed as a band insulator Hamiltonian which retains the topology of the physical insulator. Explicit examples of the entanglement spectrum are worked out, including an analytical calculation for Landau levels (similar to the work of Ref and a numerical study of three dimen-
ional topological insulators. Similar reasoning can be applied to topological superconductors. Such a relation has also been noticed in isolated examples, like the quantum Hall and the $p_x + ip_y$ superconductor edge. Independent studies have appeared, pointing to a similar connection.

Next, we consider the converse - i.e., do protected modes in the entanglement spectrum necessarily imply protected surface excitations? We show explicitly that this is not true, by studying an example of an insulator with only inversion symmetry. Here no protected surface excitations exist, but the entanglement spectrum features protected states, which points to a more subtle distinction between phases. The entanglement spectrum remains gapless because inversion symmetry is retained when dividing the system for the purposes of calculating entanglement entropy, but is implemented in a strange way, as a particle-hole symmetry of the single particle entanglement states. This leads to protected modes. Thus studying systems with inversion symmetry (or another symmetry that maps the left and right halves to one another) is a good way to break the close correspondence between edge states and entanglement, a point noticed earlier for one-dimensional interacting states in Ref. 15,16 When this correspondence breaks down, the protected entanglement degeneracies still indicate a distinct phase, although there are no physical surface states. Understanding the consequences of this hidden degeneracy should be interesting. Although disorder breaks inversion symmetry, and is hence not normally studied while classifying topological insulators, clean physical systems with inversion symmetric bulk states can certainly be realized.

Finally, we recast the theory given here in a form that is suitable for studying interacting systems: the action of inversion ($I$) is defined on the many-body Schmidt states. It is shown to act as an anti-unitary operator $IM$, which must satisfy $(IM)^2 = -1$ or $(IM)^2 = +1$. The latter corresponds to the topologically nontrivial case, and leads to a two fold degeneracy of all states in the entanglement spectrum. This degeneracy remains on introducing weak interactions. Part of the topological distinction implied by this observation is contained in the quantized magnetoelectric polarizability of insulators, which remains quantized in inversion-symmetric systems. We also discuss finer distinctions between inversion-symmetric insulators, but their physical implications remain to be identified in future research.

II. TOPOLOGICAL BAND INSULATORS

A band insulator is described by the single particle Hamiltonian:

$$H = \sum_{\gamma, k} \epsilon_\gamma (k) d^{\dagger}_{\gamma k} d_{\gamma k}$$

(2)

where $k$ is crystal momentum, and $\gamma = 1, \ldots, N$ is a band index, of which $n$ bands are filled i.e. $\epsilon_\gamma (k) < 0$ if $1 \leq \gamma \leq n$ and $\epsilon_\gamma (k) > 0$ if $n < \gamma \leq N$. The band wave-functions are:

$$d^{\dagger}_{\gamma k} = \sum_r \phi^{\dagger}_{\gamma k}(r) \psi(r),$$

(3)

where we have suppressed spin and orbital indices (These variables can be included in $r$ with the spatial coordinates).

Topological phases of band insulators are defined by their band topology. Two insulators differ topologically if they cannot be connected by smooth changes of the Hamiltonian while the band gap remains finite. It is possible to define a topological invariant to distinguish between different phases that depends only on the wave-functions of the filled bands.

Given a general band insulator, a topologically equivalent insulator can be constructed by setting the energy of all occupied bands to be equal and negative, and all unoccupied bands to be equal and positive: e.g.

$$\epsilon_{F, \gamma}(k) = -\frac{1}{2} \text{if } \gamma \leq n$$

(4)

$$\epsilon_{F, \gamma}(k) = +\frac{1}{2} \text{if } \gamma > n.$$  

(5)

Let us call the corresponding operator $\hat{Q}$. Note, this is related to the projection operator $\hat{P}$ on the filled bands via $\hat{Q} = \frac{1}{2}(1 - \hat{P})$. This “flat band” limit has been found to be useful in the classification of topological insulators and will be used here as well. An important connection is with the correlation function $C(r, r') = \langle \psi^\dagger_r \psi_{r'} \rangle$, evaluated in the ground state. Now $\hat{P} = \hat{C}$, i.e. the correlation function of the band insulator, viewed as a matrix, is simply the projection operator onto the filled bands. Hence

$$\hat{Q} = \sum_r \frac{1}{2} \psi_{r}^\dagger \psi_{r} - \sum C(r, r') \psi_{r}^\dagger \psi_{r'}.$$  

(6)

describes the flat-band insulator. Since correlations in a gapped state like a band insulator fall off exponentially rapidly with separation, the effective “flat band” Hamiltonian has essentially short ranged matrix elements, as for a physical operator. Hence, it can be viewed also as a bona fide Hamiltonian, with the same band topology as the starting Hamiltonian in Eqn. (2).

Most band insulators with nontrivial band topology are characterized by edge states. Consider representing the Hamiltonian of a band insulator in real space:

$$H = \sum_{r, r'} \mathcal{H}(r, r') \psi^\dagger_{r} \psi_{r'}$$  

(7)

$$\mathcal{H}(r, r') = \sum_{\gamma k} \epsilon_{\gamma}(k) \phi^\dagger_{\gamma k}(r) \phi_{\gamma k}(r')$$  

(8)

A boundary along the plane $x = 0$, with the physical system to the right ($x > 0$), is obtained by truncating
If both the system and the cut preserve translation symmetry, one can simultaneously diagonalize the density matrix and the translation operators parallel to the cut \(T_x, T_y\). The entanglement spectrum is then obtained as a function of momentum \(K = (K_x, K_y)\) along the cut: \(E_\alpha(K)\). This object can capture fairly detailed properties of the ground state wavefunction that are discussed in what follows.

For the case of single particle Hamiltonians, such as Eqn. \(\ref{eqn:entanglement_hamiltonian}\) Ingo Peschel has shown how to determine the entanglement Hamiltonian and its eigenvalues\(^{10}\) The first step is to realize that the entanglement Hamiltonian must be quadratic in the Fermionic operators:

\[
H^R_\alpha = \sum_{r,r'} \psi^R_r \hat{H}^R \psi^R_{r'}, \tag{13}
\]

This can be seen, and the single particle “entanglement Hamiltonian” \(\hat{H}^R\) determined, by noting that any correlation function of operators that only involve degrees of freedom on the right is unaffected by tracing out the left half of the system. For example, consider the correlation function \(C(r,r') = \langle \psi^L \psi^R \rangle\), in the ground state, before the system is cut. Now, if both coordinates \(r, r'\) belong to the right half of the system, then they are unaffected on tracing over the left half. Therefore, the same result should be obtained by using the density matrix for the right half,

\[
\text{Tr}[\rho^R \hat{\psi}^L \psi^R] = C_R(r,r') \tag{14}
\]

where \(C_R\) is the correlation function restricted to this half, namely \(C_R(r,r') = C(r,r')\) if both coordinates are on the right, and zero otherwise. A similar argument applies to multiparticle correlations. Thus, since Wick’s theorem is obeyed by correlation functions in the original uncut system, it will continue to hold for just the right half of the system in the mixed state \(\rho^R\). Consequently, \(\rho^R\) must be Gaussian, i.e. the exponential of a quadratic form of Fermion operators. Requiring also conservation of particle number leads to the general form in Eqn. \(\ref{eqn:entanglement_hamiltonian}\) An expression for \(\hat{H}^R\) may be obtained by returning to two-point correlations, and requiring that the “Boltzmann” distribution, Eq. \(\ref{eqn:boltzmann_distribution}\), gives the expression Eq. \(\ref{eqn:entanglement_hamiltonian}\). One expands the Fermion operators in a basis which diagonalizes \(\hat{H}_G^R\); in this basis, \(C\) becomes a diagonal matrix recording the mean occupation numbers of the states, given by the Fermi distribution. Thus, \(C_R = |1 + e^{-\hat{H}_G^R}|^{-1}\), or

\[
\hat{H}_G^R = \log \left[ \frac{1 - \hat{C}_R}{\hat{C}_R} \right]. \tag{15}
\]

Equivalently, the operator \(\hat{Q}_R = \frac{1}{2} \mathbf{1} - \hat{C}_R\), satisfies the relation: \(\hat{Q}_R = \frac{1}{2} \tanh[\frac{1}{2} \hat{H}_G^R]\). Thus if \(p_\alpha\) are the eigenvalues of \(\hat{C}_R\), which are readily seen to satisfy \(0 \leq p_\alpha \leq 1\), then the eigenvalues \(\epsilon_\alpha^R\) of the ‘single particle’ entangle-
ment Hamiltonian $\mathcal{H}^R$ are obtained from Eqn. 15

$$\epsilon_i^c = \log \left[ \frac{1 - p_i}{p_i} \right]$$

(16)

The many body entanglement spectrum $E_\alpha^c$ is obtained by deciding the occupancy of the single Fermion modes, so that mode $i$ has $n_i^\alpha = 0, 1$. Then $E_\alpha^c = \sum_i n_i^\alpha \epsilon_i^c$. The density matrix eigenstate with the largest eigenvalue is like the Fermi sea of a physical system; it corresponds to the lowest "energy" $E_0^c$ obtained by filling all $\epsilon_i^c < 0$.

For a translationally symmetric cut the entanglement energies can be resolved as a function of the total transverse momentum $\mathbf{K}_\perp$ (following Ref. 10). These energies can again be built from the single particle "energies" of the occupied states, $\epsilon_i^c(\mathbf{k}_\perp)$, which are functions of the momentum parallel to the cut. The total momentum $\mathbf{K}_\perp$ is also just the sum of the momenta of the filled single particle states. Thus, the fundamental object we will focus on calculating is the single particle "spectrum" as a function of transverse momentum $\epsilon_i^c(\mathbf{k}_\perp)$.

IV. CONNECTING THE ENTANGLEMENT SPECTRUM TO EDGE MODES

The previous discussion clarifies the precise connection between the entanglement spectrum and the edge spectrum of an insulator. The single particle entanglement spectrum $\epsilon_i^c(\mathbf{k}_\perp)$ is related to the spectrum obtained when a flat band version of a physical Hamiltonian is studied in the presence of an edge. The eigenvalues of the flat band Hamiltonian $\mathcal{H}$, which are $\frac{1}{2} - p_i(\mathbf{k}_\perp)$, are related to the entanglement spectrum $\epsilon_i^c(\mathbf{k}_\perp)$ via Eqn. 16, or

$$\frac{1}{2} - p_i(\mathbf{k}_\perp) = \frac{1}{2} \tanh(\frac{1}{2} \epsilon_i^c(\mathbf{k}_\perp)).$$

(17)

Most states have eigenvalues $\epsilon_i \to \pm \infty$, because of the nonlinear relationship; the eigenvalues of $\mathcal{C}$ in the bulk are 1 and 0. Very negative eigenvalues represent bulk states that are occupied, and large positive eigenvalues represent unoccupied states.

In cases where topologically protected surface states of the physical Hamiltonian are expected, the flat band deformation which is topologically equivalent is also expected to have surface states, filling the whole gap between the bulk states at $+\infty$ and $-\infty$.

Note however, the converse is not necessarily true. For inversion symmetry (see below), the edge of the flat band Hamiltonian has structure which signifies protected features of a phase, although this structure is not present in the physical surface states of a generic Hamiltonian in the same topological class.

We will now illustrate our reasoning with various examples.

V. EXAMPLES

Let us summarize the procedure for obtaining the entanglement spectrum. The following prescription takes advantage of $\mathbf{k}_\perp$ conservation to reduce the problem to a one-dimensional problem: (i) obtain the correlation function restricted to the right half, by summing over occupied bands. If the wavefunction of the filled orbitals at momentum $\mathbf{k} = (k_x, \mathbf{k}_\perp)$ is $\phi_{ik} e^{i\mathbf{k}_\perp \cdot \mathbf{r}}$, where $\mathbf{r}$ is the unit cell position, and $a$ refers to other indices such as sublattice and spin, then:

$$C^R_{\mathbf{k}_\perp}(x, a; x', a') = \sum_{i, k_x} e^{i k_x (x-x')} \phi^*_{ik}(a') \phi_{ik}(a).$$

(ii) Find $C$’s eigenvalues $p_i(\mathbf{k}_\perp)$, by solving the eigenvalue equation

$$\sum_{x' a'} C^R_{\mathbf{k}_\perp}(x, a; x', a') f^R_{ik}(a') = p^R(\mathbf{k}_\perp) f^R_{ik}(x, a)$$

(iii) Then the single particle entanglement spectrum $\epsilon_i^c(\mathbf{k}_\perp)$ can be read off from equation (17) and the eigenfunctions are $f_{ik}(x) e^{i\mathbf{k}_\perp \cdot \mathbf{r}}$. We will graph our results for $\frac{1}{2} - p^R(\mathbf{k}_\perp)$ instead of $\epsilon_i^c(\mathbf{k}_\perp)$, since they are monotonically related.

A. Integer Quantum Hall:

The first example is based on the work of Ref. 11 on the integer quantum Hall effect. This is an especially clear illustration of the general relationship between the correlation function and the entanglement Hamiltonian. Consider electrons confined to a plane and in a strong magnetic field; assume there is no crystal potential and suppose that exactly $\nu$ Landau levels are fully occupied. We show that the entanglement spectrum contains the expected $\nu$ chiral edge modes. Using the Landau gauge, $A_y = Bx$, and labeling the states by the momentum along the cut $k_x = k_y$, the restricted correlation function is given by:

$$C^R_{\mathbf{k}_x}(x, x') = \sum_{n=1}^{\nu} \phi^*_{nk}(x') \phi_{nk}(x)$$

where the normalized eigenstates are $\phi_{nk}(x) = H_n(X - Bx)$.
\(K_y) e^{-(X-K_y)^2/2}; \) here \(X = x/l; \) \(K_y = k_y/l\) are dimensionless variables scaled by the magnetic length \(l = \sqrt{\hbar/eB},\) and \(H_n\) are appropriately normalized Hermite polynomials.

Now, an eigenfunction of \(C_{k_y}^R\) must be constructed from linear combinations of the Landau level states \(f^a = \sum_{m=1}^{\nu} c_m \phi_m(\nu)\) (where \(k_y\) has been suppressed). The coefficients \(c_m\) are easily seen to be eigenvectors of the \(\nu \times \nu\) matrix \(F_{nm}(k_y) = \int_0^\infty dx \phi_{nk_y}(x) \phi_{mk_y}(x)\). For \(\nu = 1\), this is a number, which is the eigenvalue itself. Thus

\[
1/2 - p_0(k_y) = -\frac{1}{2} \text{erf}(K_y),
\]

which interpolates between \(-1/2\) (when \(k_y = -\infty\)) and \(+1/2\) (when \(k_y = +\infty\)). This is the single chiral mode, as expected. Similarly, the \(\nu = 2\) case can be solved analytically, the result for the two eigenvalues is now

\[
\frac{1}{2} - p_{1, 2} = -\frac{1}{2} \text{erf}(K_y) - e^{-K_y^2} \left( \frac{K_y}{2\sqrt{\pi}} \pm \sqrt{\frac{2 + K_y^2}{\pi}} \right),
\]

leading to two modes as shown in the figure. These two modes are like the dispersion of two chiral particles in a one-dimensional system. In general, the entanglement Hamiltonian of a gapped system behaves like the Hamiltonian of a system with one dimension fewer. There may be infinitely many bands besides those near \(\epsilon^c = 0\), but their energies rapidly approach \(\pm \infty\).

**B. Three Dimensional Topological Insulator with Time Reversal Symmetry:**

We now compare the physical surface states that appear in this model and the entanglement spectrum of a cut with the same orientation. We choose a surface normal to the (1,1,1) direction so as to cut bonds with strength \(t\) for three of the bonds, and \(t+\delta t\) for the fourth bond oriented along the (-1,1,1) direction. To access a generic Hamiltonian we also include regular second-neighbor hopping \(t_2\) (not shown in Eq. [18]) in all directions. The spin orbit interaction \(t_{SO}\) appears in the second term, inducing hopping between second neighbor sites. In this term, \(d_{ik}^1; d_{ik}^2\) are the two nearest neighbor bond vectors leading from site \(i\) to \(k\), and \(\sigma\) are the spin Pauli matrices. This model respects time reversal symmetry, and also inversion symmetry (i.e.

\[
1/2 - p_0(k_y) = -\frac{1}{2} \text{erf}(K_y),
\]

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**B. Three Dimensional Topological Insulator with Time Reversal Symmetry:**

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obtained. The node is centered at the time reversal invariant $M2$ point of the surface Brillouin Zone (BZ) (see Figure 6(a)). This is selected by the direction of the strong bond $t + \delta t$. Note that the surface spectrum is not symmetric between positive and negative energies, as it would be if the model were particle-hole symmetric.

Below, in Figure 6(b), we display the two surface eigenvalues of the single particle entanglement spectrum $\epsilon_i^e(k_\perp)$, obtained from the ground state of the Hamiltonian in Eqn. (15) by dividing the system into two halves. The plane that divides the system is oriented in the same way as the physical boundary previously discussed. It is more convenient to display $\frac{1}{2} \tanh(\frac{\epsilon_i^e(k_\perp)}{2})$ which is related to the eigenvalues $p_i(k_\perp)$ of the correlation function $C_R$ via $\frac{1}{2} \tanh(\frac{\epsilon_i^e(k_\perp)}{2}) = \frac{1}{2} - p_i(k_\perp)$. Note zero "energy", $\epsilon_i^e(k_\perp) = 0$, also corresponds to the zero of $\frac{1}{2} - p_i$. Clearly, we see that the entanglement spectrum also displays the same characteristics as the protected surface modes. There is a single Dirac cone which is centered at the same point in the surface BZ as the surface state itself. The "energy" of this Dirac cone is curiously zero (understanding this is our next job).

Similarly, if we choose $\delta t < 0$, we obtain a weak topological insulator, whose physical surface states and entanglement spectrum are compared in Figure 5 for the same surface as above. Again, the Dirac nodes of the physical surface states, and their location in the Brillouin zone, which are fixed by band topology, are captured by the entanglement spectrum.

We now briefly describe the computation that gives us the entanglement spectrum in the figures. Essentially, we follow the three step procedure outlined in Section VI. To identify insulators of this type.

We now discuss the origin of Fig. 6, where a perturbation breaking time-reversal symmetry has been added. The entanglement spectrum still has a Dirac node, which is in fact at zero entanglement "energy", although the surface states are gapped. Therefore, while a system with topologically protected surface states also has topologically protected entanglement states, the converse may not be true. The Dirac node is a feature in the entanglement spectrum of inversion symmetric insulators, which defines a distinct phase, although there are no topological surface states for the physical Hamiltonian generally. The entanglement spectrum is an especially useful tool for identifying insulators of this type.

VI. TOPOLOGICAL INSULATORS WITH ONLY INVERSION SYMMETRY

We now discuss the origin of Fig. 6 where a perturbation breaking time-reversal symmetry has been added. The entanglement spectrum still has a Dirac node, which is in fact at zero entanglement "energy", although the surface states are gapped. Therefore, while a system with topologically protected surface states also has topologically protected entanglement states, the converse may not be true. The Dirac node is a feature in the entanglement spectrum of inversion symmetric insulators, which defines a distinct phase, although there are no topological surface states for the physical Hamiltonian generically. The entanglement spectrum is an especially useful tool for identifying insulators of this type.
FIG. 6: Inversion symmetric insulators with broken time reversal symmetry. Note the physical states (a) are gapped, but the Dirac node remains in the entanglement spectrum (b).

The reason the entanglement spectrum works for identifying phases with inversion symmetry, while physical surface states fail, is as follows. A physical boundary necessarily breaks inversion, since inversion maps the insulator to its exterior. But now consider a cut that passes through a center of inversion. The inversion $I$ relates the left and right sides of an entanglement cut. This inversion symmetry leads to a symmetry of the entanglement Hamiltonian, but with the twist that it is realized as a sort of particle-hole symmetry for the two dimensional entanglement spectrum (see also Refs. 15,16).

Let us suppose that the inversion symmetric cutting plane does not exactly coincide with any orbitals (so that it divides the states into separate parts)\textsuperscript{28}. We call the inversion transformation through the center of inversion on the plane $I$. In this section, we will describe how this symmetry constrains the entanglement states, then use this to prove the stability of the entanglement Dirac node. Finally we discuss what physical difference could be embodied in this topologically distinct entanglement spectrum. The remaining sections will discuss interacting insulators.

To see why inversion symmetry acts as a particle-hole symmetry we will give an additional interpretation of the entanglement eigenstates $f^R_{i\mathbf{k}_\perp}$. The entanglement spectrum can be understood most intuitively by showing that a set of wave functions for the full system\textsuperscript{22,23}

\begin{equation}
F_{i\mathbf{k}_\perp}(x, r_\perp) = \left[ \sqrt{p_i(\mathbf{k}_\perp)}f^R_{i\mathbf{k}_\perp}(x) + \sqrt{1-p_i(\mathbf{k}_\perp)}f^L_{i\mathbf{k}_\perp}(x) \right] e^{i\mathbf{k}_\perp\cdot r_\perp}
\end{equation}

can be constructed, satisfying two properties: first, the $f^R$'s and $f^L$'s form an orthonormal family of wavefunctions in the two halves. Second, filling all the states $F_{i\mathbf{k}_\perp}$ gives the band insulator; i.e. they can be thought of as being obtained from the filled band wavefunctions (Eq. 8) by a unitary transformation. The $f^R$'s and the $p_i$'s turn out to be the same as before. (See the appendix.) The eigenvalues $p_i(\mathbf{k}_\perp)$ have a simple interpretation in light of Eq. (19). Each state $F_{i\mathbf{k}_\perp}$ is certainly occupied by an electron in the band insulator. The eigenvalue $p_i(\mathbf{k}_\perp)$ represents the probability that the electron in this state is found on the right half. For example, when $p_i \approx 1$, corresponding to $\epsilon_i \to -\infty$, the electron in $F_i$ is almost certainly on the right half. This fits with the previous definition of the $f^R$'s because $\epsilon_i$ is far below the “Fermi energy,” so the $i$th state is occupied in the “Fermi sea” of the entanglement Hamiltonian. Eqn. (19) leads to a very intuitive way of understanding the entanglement spectrum, as reviewed in appendix A.

Because of the inversion symmetry, there is a map $I_S$ on the single-particle states that takes a state $f^R_{i\mathbf{k}_\perp}$ to another state $f^R_{i-\mathbf{k}_\perp}$. This state flips the sign of the en-

FIG. 7: Without inversion symmetry. Both the physical surface state (a) and the entanglement spectrum (b) are gapped.
tanglement energy, $\epsilon_f^\dagger(-k_\perp) = -\epsilon_f^\dagger(k_\perp)$. The mapping arises directly from inversion symmetry acting on the $F$’s (see Fig. 8), which produces from any occupied state $F_i$ with momentum $k_\perp$ a second state, $F_i$, with the opposite momentum:

$$F_{-k_\perp}(x, r_\perp) = F_{ik_\perp}(-x, -r_\perp).$$

(20)

Expanding this equation gives

$$\left[\sqrt{p_i(-k_\perp)} f^R_{i-k_\perp}(x) + \sqrt{1-p_i(-k_\perp)} f^L_{i-k_\perp}(x)\right] e^{-ik_\perp r_\perp}$$

$$= \left[\sqrt{p_i(k_\perp)} f^R_{ik_\perp}(-x) + \sqrt{1-p_i(k_\perp)} f^L_{ik_\perp}(-x)\right] e^{-ik_\perp r_\perp}.$$  

Since inversion maps the left-hand side to the right-hand side, these equations imply that $p_i(-k_\perp) = 1 - p_i(k_\perp)$ and that $f^R$ is obtained from a state on the other side of the partition, namely $f^R_{i-k_\perp}(x) = f^L_{ik_\perp}(-x)$. Using the relation between $p$ and $e$, it follows that a mode with “energy” $e^f$ and momentum $k_\perp$, is mapped by inversion to one with $-e^f$ and $-k_\perp$. A more algebraic proof of this result is in Appendix A.

Having established the action of inversion, we now turn to the stability of Dirac modes in the entanglement spectrum, in the presence of inversion. Suppose the insulator is obtained from a time-reversal symmetric topological insulator by applying a time reversal breaking perturbation. (We plan to derive the basic properties of general inversion symmetric insulators later.) A Dirac mode in the entanglement spectrum (or physical surface spectrum) occurs at a time reversal invariant momentum (or TRIM) $k_\perp$. These momenta are half of a reciprocal lattice vector, i.e., $k_\perp \in \{\Gamma, M1, M2, M3\}$, so that $k_\perp = -k_\perp$ (modulo the reciprocal lattice).

First consider the modes in the unperturbed crystal, that is both time-reversal and inversion symmetric. At the tip of the cone of a Dirac mode, there are two degenerate states $f^R_{k_\perp}$, $f^L_{k_\perp}$. These must have $e^f = 0$, because otherwise applying $I_S$ would produce a second Dirac point at $-e^f$.

Now the symmetry $I_S$ ensures that these Dirac modes have to remain at zero “energy” when time-reversal symmetry is broken by a small perturbation. First, the two states are transformed into themselves under $I_S$, so appropriate linear combinations of them are inversion eigenstates. In fact, their inversion parities must be the same. (The states formed a Kramers doublet under time-reversal symmetry before it was broken.) Therefore the states $f^R_{k_\perp}$ and $f^L_{k_\perp}$ cannot evolve into a pair $f^R_{-k_\perp}$, $f^L_{-k_\perp}$ with energies $\pm e^f$, without a discontinuous jump in the inversion parities. (Inversion symmetry interchanges these new states, so their combinations $\sqrt{1/2}(f^R_{k_\perp} \pm f^L_{k_\perp})$ have opposite parities.)

Note, in general, the spectrum consists of equal numbers of states that are even under inversion and odd under inversion. All the pairs of states at nonzero entanglement energy can be combined into pairs of states of opposite parity, since $f_{i-k_\perp} \rightarrow f_{i-e^f-k_\perp}$, and one can take symmetric and antisymmetric combinations of these. The only exceptions are states at zero energy located at a TRIM. These are actually the tips of Dirac nodes in the case at hand. Thus, $\Delta \nu_{k_\perp}$, the difference between the number of even and odd states at the TRIM $k_\perp$ is the number of unapplicable states. Therefore, $\Delta \nu_{k_\perp}$ cannot change except at a phase transition of the bulk crystal, where the entanglement spectrum becomes ill-defined or changes discontinuously. At a second order transition, in particular, this topological invariance breaks down because the entanglement Hamiltonian, Eqn. [4], has long-range hopping and infinitely many bands (including the bulk bands) collapse to zero energy (in analogy with the observations of Ref. [22]). The states may then all mix together. We will assume here that the unapplicable states all come in Dirac pairs, so $\Delta \nu_{k_\perp}$ is even.

FIG. 8: Inversion symmetry of entanglement. (a) The transformation $I_S$ of single-body modes. The image of a state $f^R$ under $I_S$ is not defined on the merits of $f^R$ itself (like ordinary reflection), but instead depends on the state of the system. The extended wave function $F_i = \sqrt{p_i} f^R_i + \sqrt{1-p_i} f^L_i$ is inverted, and $I_S f^R$ is (up to normalization) the right-hand part of this, which can look completely different from the original $f^R$. (b) The transformation $M_L$ of many-body states in a non-interacting system. Each term in the Schmidt decomposition is obtained by placing electrons on either the right or left of the $F_i$’s indicated by the horizontal lines. Inversion is applied to the system as a whole. Focusing just on the half right-hand side of the system, one finds that inversion induces a particle-hole like transformation ($M_L$) because levels $i$ that are occupied in $|\chi_R\rangle$ correspond to empty levels $i$ in $M_L|\chi_R\rangle$. 


The parity argument shows that there is a distinct phase of inversion symmetric insulators defined by having a protected Dirac dispersion in the entanglement spectrum. What physical property distinguishes this phase? Clearly, surface states are not the answer since all physical surface states are gapped. At least one distinction is captured by the electromagnetic response of the system.\(^{20}\) Consider integrating out the Fermions in the presence of weak external electromagnetic fields. Then the effective action contains a term:

\[
S_\theta = i\theta \frac{e^2}{2\pi \hbar} \int d\tau d^3 x \mathbf{E} \cdot \mathbf{B},
\]

Inversion symmetry and time reversal symmetry each imply that \(\theta\) is quantized in units of \(\pi\). Under time reversal, the sign of this term is changed since \(\mathbf{B} \rightarrow -\mathbf{B}\). However, this does not rule out \(S_\theta\). The reason is that \(S_\theta\) contributes a factor of \(e^{-2\pi i \theta}\) to the weight of a field configuration in the path integral. The term in square brackets is an integer for periodic boundary conditions in space and imaginary time, so \(\pi + \theta + 2\pi\) are physically equivalent. Hence effects due to \(S_\theta\) are time reversal invariant as long as \(\theta\) is 0 or \(\pi\). Note furthermore that if the system only possesses inversion symmetry in the bulk, then one can argue instead that the sign of this term changes because \(\mathbf{E} \rightarrow -\mathbf{E}\) under inversion.

The nonzero value, \(\theta = \pi\), is realized in strong topological insulators, time-reversal symmetric systems with an odd number of surface Dirac nodes.\(^{20}\) It is therefore natural also to suppose that an insulator with an odd number of entanglement nodes, but with only inversion symmetry, has an electromagnetic response of \(\theta = \pi\). (This remains true even for inversion symmetric insulators that cannot be obtained by perturbing time-reversal symmetric insulators.\(^{23}\)) Note, the entanglement spectrum gives us a very simple way to predict how the insulator responds to an electromagnetic field based solely on ground state properties.

The physical meaning of \(S_\theta\) is that applying a magnetic field induces a parallel polarization of charge of magnitude \(\theta \frac{e^2}{2\pi \hbar} \mathbf{B}\). Measuring this sharply is challenging, but it is at least in principle a physical consequence of the entanglement nodes. The locations and numbers of nodes are also invariant, at least without interactions, but we do not know the physical consequences of these properties.

### VII. STABILITY AGAINST INTERACTIONS

Thus far, we have discussed topological properties of systems without interactions. An interesting question is how many of the topological distinctions remain when the interactions between electrons are taken into account. When surface states exist, one can determine whether interactions affect their properties by studying whether the interactions are “relevant perturbations” to the field theory of the Dirac modes.\(^{24}\) Furthermore, the bulk magneto-electric polarizability remains quantized even when interactions are included. But the entanglement spectrum remains gapless even when there are no surface states and captures quantum numbers not accounted for by \(\theta\); at the very least, we believe the values of \(\Delta \nu_{a\perp}\) are conserved modulo 2 at each transverse TRIM. (Similar invariants can be constructed for each direction of the entanglement cut, but presumably only a few of these are independent.)

To describe inversion symmetry in an interacting state, one must understand how it acts on the \(\text{many body}\) states appearing in the Schmidt decomposition. Inversion turns out to be related to an \(\text{anti-unitary}\) operator, \(\ket{\mathcal{R}} \rightarrow \mathcal{M} \mathcal{T} \ket{\mathcal{R}}\). The action of this symmetry is most interesting when restricted to the even-split Schmidt states, where half the \(N\) particles are on each side of the divider. Here, it satisfies \((\mathcal{M} \mathcal{T})^2 = -1\) when there are an odd number of Dirac nodes. Thus, inversion behaves exactly like the Kramers transformation, and each Schmidt state is doubly degenerate even with interactions included. Interestingly, Fermion \(\text{anticommutation}\) is a key ingredient in establishing this fact. It has been shown recently\(^{13,10}\) that inversion acts on one dimensional Haldane chains in a similar way.

#### A. Many Body States and Inversion Symmetry

Consider the action of inversion symmetry \(\mathcal{I}\) on the many body Schmidt states

\[
\ket{\Psi_G} = \sum_a e^{-E_a^R/2} \ket{\Phi_a^R} \ket{\Phi_a^L},
\]

Inversion maps a right-hand state to a left-hand one. Since this is a symmetry, the two must have the same entanglement eigenvalue \(E_a^R\). Thus, if each eigenvalue has a non-degenerate eigenstate, the inversion transformation is simple: each state maps to its partner (up to a phase). Things get more interesting when degenerate states are present in the entanglement spectrum.

Consider a multiplet of even-split states \(\ket{\Phi_a^R}\), where we use the label \(a = 1,\ldots,d\) to label the \(d\) degenerate states in the Schmidt basis above, Eq. (22). Its image under inversion is a linear combination of states on the left:

\[
\ket{\Phi_a^R} \rightarrow \sum_{b=1}^{N} I_{ba} \ket{\Phi_b^L}
\]

If inversion is to be viewed as a symmetry, we need to return to the right portion of the system, to make statements about the entanglement eigenstates of a single subsystem. (See Fig. [3].) (Symmetries mapping systems to one another are not so useful—for example knowing that the mirror image of a left-handed molecule is a right-handed molecule does not imply that the orbitals associated with one of these molecules have special symmetry.) Inversion can be converted to a symmetry of one part using the pairing of left and right states in the Schmidt
decomposition \(^{22}\). This pairing is described by a transformation \(M\) which maps \(|\Phi_L^a\rangle\rightarrow |\Phi_R^b\rangle\). This rule can be extended consistently to an antilinear transformation on the rest of the Hilbert space for the left side of the system.

To see this, let us describe the partner of a general state \(|\chi^L\rangle\) on the left in a basis-independent way:

\[
M|\chi^L\rangle = \langle \chi^L | \rho_R^{-\frac{1}{2}} | \Psi_G\rangle. \tag{24}
\]

The right-hand side is a partial inner product. It is not a number but a wave function for the right half of the system since only the degrees of freedom on the left half are summed over:

\[
M|\chi^L\rangle = \sum_{\{a^L\}} \Psi_G(\{a^L\}, \{a^R\}) \chi^L(\{a^L\})|\{a^R\}\rangle.
\]

where \(\{a^L\}, \{a^R\}\) are the variables describing the two halves. Note that this is antilinear in \(|\chi^L\rangle\) because of the complex conjugation. Now, \(|\chi^L\rangle = \sum_i c_i |\Phi_i^a\rangle\) is mapped by this transformation to \(|\sum_i c_i^* |\Phi_i^R\rangle\rangle\). Each Schmidt state, in particular, maps to its partner. Briefly, Eq. (24) utilizes the ground state to connect the left and right halves, and the operator \(\rho_R^{-\frac{1}{2}}\) is there to strip off the different Schmidt weights.

Now the combination of \(M\) and \(I\) is a stand-in for inversion symmetry that returns states on the right-hand side of the cut back to the right-hand side; in the basis of Schmidt states, this transformation is represented by \(KI\) where \(K\) is complex conjugation and \(I\) is the matrix given above.

When \(MI\) is performed twice, the state must return to itself, modulo a phase, hence

\[
II^* = 1 e^{i\phi}. \tag{25}
\]

This phase factor can be only \(\pm 1\) because it has to be real\(^{23}\). More precisely, the operator \((MI)^2\) has to have the same value \((-1)^3\) for each Schmidt state which has half the electrons on each side, since the wave function Eq. (1) is a parity eigenstate (see Appendix \(B\)).

The case \(I 
 I^* = -1\) is specially interesting. Time reversal symmetry of spin 1/2 + \(n\) particles has the same property, which can be used to prove Kramers’ degeneracy. This algebra has no one-dimensional representation. (If \(I\) is a c-number, the product is nonnegative.) A two dimensional representation is exemplified by \(I = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\), the antisymmetric matrix. Since this is actually the generic case, whenever the inversion operator in a particular system obeys this algebra, all levels must be at least doubly degenerate.

We now show that this is indeed how the inversion operator acts in the even-split states when there is an odd number of Dirac nodes, by showing that \(\delta\) is the number of Dirac nodes modulo 2. For states \(|\Phi_R\rangle\) with \(N + k\) Fermions on the right side, \((MI)^2\) can be different, but there will still be entanglement degeneracies if \(k \neq 0\); the entanglement eigenvalues for positive and negative \(k\) always match, since the Schmidt state \(|\Phi_R\rangle\) is degenerate with \(|I\Phi_L\rangle\) (and has the opposite \(k\)). This relation (valid for any inversion-symmetric insulator) is not as interesting as the degeneracies among the states with the same value \(k = 0\), which is unique to topological insulators.

### B. Inversion and the Topological Insulator

We now determine the value \(II^* = \pm 1\) for topological insulators in the noninteracting limit. Note, this also allows us to make statements about the interacting case, since the value cannot jump when small interactions are introduced.

The ground state of the noninteracting system can be built up by creating particles in all the modes \(F_l\) (see Eq. \(19\)). Suppose there is just one Dirac node. Then

\[
|\Psi_G\rangle = \frac{1}{2} (r^\dagger_a + l^\dagger_a)(r^\dagger_b + l^\dagger_b) \times \prod_{l_{k\perp} \text{even}} (\sqrt{p_l(k_{\perp})} r^\dagger_{l_{k\perp}} + \sqrt{1 - p_l(k_{\perp})} l^\dagger_{l_{k\perp}}) \times \prod_{l_{k\perp} \text{odd}} (\sqrt{p_l(k_{\perp})} r^\dagger_{l_{k\perp}} + \sqrt{1 - p_l(k_{\perp})} l^\dagger_{l_{k\perp}}) |0\rangle \tag{26}
\]

\[
r^\dagger_{l_{k\perp}} = \sum_r e^{i k_{\perp}} r f^L_{l_{k\perp}}(r)\psi(r)^\dagger \tag{27}
\]

\[
l^\dagger_{l_{k\perp}} = \sum_r e^{i k_{\perp}} r f^R_{l_{k\perp}}(r)\psi(r)^\dagger. \tag{28}
\]

where the first two factors are the Dirac node states. Expanding Eq. (26) gives the Schmidt decomposition. One should convince oneself of the following relation between the many-body transformations \(MI\) and the one body implementation of inversion, \(I_S\): if \(|\chi_R\rangle\) is one of the Schmidt states, and \(f^R\) is occupied in this state, then \(I_S f^R\) is empty in \(\sum I_M |\chi_R\rangle\) (see Fig. 8b).

Note that the second line of Eq. (26) contains the states that are mostly on the right, and the third contains those mostly on the left. Inversion maps these states to one another. The two states at the Dirac node are inversion eigenstates, so they map to themselves. Since they also have the same parity (say they are even, for instance), \(r_{a,b} \leftrightarrow l_{a,b}\).

The highest weight states in the Schmidt decomposition of the wavefunction involve acting with \(r^\dagger_a\)’s when \(p_l > 1/2\) and with \(l^\dagger_a\)’s when \(p_l < 1/2\), so these states are contained in

\[
\frac{1}{2} (r^\dagger_a + l^\dagger_a)(r^\dagger_b + l^\dagger_b) |S_R\rangle |S_L\rangle \tag{29}
\]

where \(|S_R\rangle\) and \(|S_L\rangle\) are the filled Fermi seas (all negative single particle entanglement energies occupied) for the two sides, which are exchanged by \(I\).

Among the highest weight states, consider the two states

\[
|\text{pair}\rangle = r^\dagger_a l^\dagger_b |S_R\rangle |S_L\rangle + l^\dagger_a r^\dagger_b |S_R\rangle |S_L\rangle
\]
with an equal number of Fermions in the two sides. While these are converted into each other under inversion, it seems possible that they could mix and split, and give rise to one dimensional representations of the inversion operation. This is where showing that the inversion matrix $I$ satisfies $I^* = -I$ comes in handy.

We can get $| \text{pair} \rangle$ into the form of the Schmidt decomposition if we define the states:

$$| \Phi_1^R \rangle = r_a^+ | S_R \rangle \quad | \Phi_1^L \rangle = l_b^+ | S_L \rangle$$

$$| \Phi_2^R \rangle = -r_a^+ | S_R \rangle \quad | \Phi_2^L \rangle = l_b^+ | S_L \rangle.$$

The ground state can be written as the Schmidt sum:

$$| \Psi_0 \rangle = \frac{1}{2} (| \Phi_1^R \rangle | \Phi_1^L \rangle + | \Phi_2^R \rangle | \Phi_2^L \rangle) + \ldots$$

(The sign $s$ in front is an unimportant sign due to Fermi statistics; see appendix [B].

Inversion maps

$$| \Phi_1^R \rangle \rightarrow | \Phi_2^L \rangle$$

$$| \Phi_2^R \rangle \rightarrow -| \Phi_1^L \rangle.$$

$\mathcal{M}$ simply maps $| \Phi_{1,2}^R \rangle$ to $s| \Phi_{1,2}^L \rangle$, so the inversion matrix is $I^* = \begin{pmatrix} 0 & -s \\ s & 0 \end{pmatrix}$. Note that the crucial minus sign has arisen because of anticommutation of Fermion operators.

Now we see explicitly that the inversion matrix satisfies $I \cdot I^* = -I$, and hence the states remain two fold degenerate. As mentioned above, this result persists for any state with equal numbers of Fermions on the two sides. When interactions are included, the even-split states all mix to-gether, but interactions are included, the even-split states all mix to-

When interactions are included, the even-split states all mix together, but interactions are included, the even-split states all mix to-

For a more general topological insulator, one can show that $I \cdot I^* = (-\delta) \hat{1}$ where $\delta$ is the number of pairs of equal-parity single-body states with $\epsilon^s = 0$, i.e. the number of Dirac nodes.

\textbf{C. Distinctions Preserved by Interactions}

Now we can argue that some distinctions among insulators survive the introduction of interactions. While this will include the quantized electromagnetic response of inversion symmetric insulators,[23] which by virtue of being a response function remains well defined in the interacting case, more other mysterious distinctions are also found. Without interactions, $\frac{1}{2} \Delta \nu_{k_z}$ is a fixed integer for each TRIM. With interactions, we will give an argument that suggests that at least the number of Dirac nodes at each $\kappa_z$, $\frac{1}{2} \Delta \nu_{k_z}$, is well-defined modulo 2 in an inversion symmetric insulator. In particular, the location of a single surface Dirac node in the Brillouin zone survives the introduction of interactions, as argued below.

The analogous quantity in the time reversal invariant insulator is the “weak” index,[14] which can be determined from the surface states or metallic topological defects in the crystal[23]. No analogous physical consequence seems available when time reversal is broken but inversion is retained.

These distinctions can be found by looking at a sample with a finite cross-section in the $y-z$ direction (but infinite in the $x$-direction, perpendicular to the cut). We have just seen that, in a noninteracting insulator, the par-ties of the zero-energy single-body states determine whether there are many-body degeneracies. Only the Dirac modes at certain TRIMs will satisfy the boundary conditions, and thus the value of $(\mathcal{M} \mathcal{L})^2$ will count the number of nodes at these TRIMs.

Say the cross-section is odd $\times$ odd, with $2N_y + 1 \times 2N_z + 1$ unit cells. Assuming periodic boundary conditions, the allowed transverse momenta will be $(\frac{2\pi n_y}{2N_y+1}, \frac{2\pi n_z}{2N_z+1})$ (where $n_y$, $n_z$ are integers whose magnitudes are less than or equal to $N_y$, $N_z$ respectively). The only one of these which is exactly time-reversal invariant is $(0,0)$. Thus all states come in pairs related by inversion symmetry except for unpaired states $\frac{1}{\sqrt{2}} (l_{a,b}^1 + r_{a,b}^1)$ at zero momentum. Therefore $\delta$ is equal to $\frac{1}{2} \Delta \nu_{(0,0)}$ and there is a double degeneracy if this is odd.

To isolate another TRIM, introduce antiperiodic boundary conditions along one or both of the other directions. (Antiperiodic boundary conditions along $y$, for example, force $k_{y\perp}$ to have the form $\frac{2\pi(n_y+1/2)}{(2N_y+1)}$, allowing $\pi$ but not $0$.) Then double degeneracy occurs when the number of modes at the new TRIM is odd.

It is possible that the actual integer value of the $\Delta \nu$’s is conserved also when interactions are introduced, but there might be a more surprising classification of interacting phases. Refs.[23],[24] gave an example for one-dimensional interacting topological insulators showing that an integer property of topological phases can be changed (by multiples of 8, in fact) when interactions are included.

\textbf{D. The Parity of the Many-body Wavefunction}

Many phases (like the ordered phase of an antiferromagnet) have a sharp distinction only for infinitely large systems, but it is possible to check what phase an inversion-symmetric insulator is by looking at a finite piece of it, with an appropriate geometry.

For a sample with periodic boundary conditions in the $y$ and $z$ directions, a finite size in the $x$-direction, and perfect inversion symmetry between its two free surfaces, $\frac{1}{2} \Delta \nu_{(0,0)} + \frac{N}{2}$ is the parity of the many-body wave-function $\psi(r_1, \ldots, r_N)$ under $r \rightarrow -r$. This can be seen when $\Delta \nu_{(0,0)} = 1$ by inverting Eq. (29): the two modes corresponding to the Dirac node just map to themselves under inversion symmetry while $| S_R \rangle$ and $| S_L \rangle$ switch places. Switching them back leads to a fac-
tor of \((-1)^{N/2-1}\) because \(N/2 - 1\) pairs of electrons have been exchanged. (See Appendix B for more details.) This parity is not any easier to measure experimentally than degeneracies in the entanglement spectrum; a measurement would require some sort of interference experiment on a macroscopic crystal\(^{\text{[6]}}\). It is just an interesting interpretation for \(\Delta\nu_{(0,0)}\). (The \(\Delta\nu\)'s at other TRIMs are related to the parities of samples with other boundary conditions.)

To check what phase a sample is in if it is not inversion symmetric, the system has to be very large. In this case, one has to use the entanglement spectrum to determine the phase, and this works only when the surfaces are far enough from the cut surface that inversion is an accurate symmetry of the entanglement surface states.

As an aside, this implies a surprising relationship between the magnetoelectric susceptibility and the parity when inversion is a symmetry: the electron-wave function of a crystal with a half-integer susceptibility is odd under inversion for the following geometry: the sample must have an even \times \text{even} cross section and periodic boundary conditions in the \(y - z\) direction. (For the even \times \text{even} cross sections all the TRIMs contribute to the parity.)

VIII. CONCLUSIONS

We have studied the entanglement spectrum of insulators with non-trivial band topology. Whenever a physical edge or surface state is present, the entanglement spectrum also is characterized by protected features. Although this is purely a ground state property, we showed it can be formally mapped to the edge spectrum of a “flat band” version of the physical Hamiltonian.

On the other hand, the converse of this is not true. Protected features of the entanglement spectrum may occur in systems that do not possess physical surface states. This can happen when a physical surface necessarily breaks an underlying symmetry of the bulk solid - for example inversion symmetry. In these cases the entanglement spectrum provides a unique perspective on classifying the phase. We illustrated this by studying three dimensional insulators with inversion symmetry. In general, no surface modes occur in these systems. However, since the entanglement cut still preserves inversion symmetry, the action of inversion on the entanglement eigenmodes can be worked out. These were shown to lead to the protected entanglement spectrum.

An advantage of defining the phase in terms of protected properties of its entanglement spectrum is that it allows us to deduce properties that remain stable when interactions are present. For the case of inversion symmetric insulators, characteristic properties beyond the quantized magnetoelectric polarizability appear to be present and are stable when the particles are interacting. The corresponding physical consequences remain to be identified.

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Appendix A: Inversion Symmetry in Noninteracting Entanglement Spectra

The transformation \(I_S f^R_{i,k_x} \to f^R_{1-i-k_x}\) can be expressed in terms of the correlation function \(\hat{C}\). First, we will show how to construct the paired functions \(F_{i,k_x}(x)\). (We will omit the \(y\) and \(z\) dependence.) Let us split the wave function into two parts, \(x > 0\) and \(x < 0\), which can be regarded as the top and bottom halves of state-vectors. Then the correlation function has four parts,

\[
\hat{C} = \begin{pmatrix} \hat{C}_R & \hat{C}_{LR} \\ \hat{C}_{LR} & \hat{C}_L \end{pmatrix}.
\]

Since \(\hat{C}\) has 1 and 0 as eigenvalues, \(\hat{C}^2 = \hat{C}\), giving four matrix equations. The equation of relevance is \(\hat{C}_{LR}(1 - \hat{C}_R) = \hat{C}_L\hat{C}_{LR}\). Given an eigenfunction \(f^R_i\) of \(\hat{C}_R\) with eigenvalue \(p_i\) one can obtain an eigenvector of \(\hat{C}_R\) with eigenvalue \(1 - p_i\) via the transformation \(M\)

\[
f^L_i(x) = [\hat{M} f^R_i](x) = \frac{1}{\sqrt{p_i(1 - p_i)}} \sum_{i > 0} \hat{C}_{LR}(x,x')\phi^R_i(x').
\]

The prefactor is inserted to ensure that \(f^L_i\) is normalized. (One can check that \(\hat{M}\) is a unitary transformation, which can be written in matrix form \(\hat{M} = \frac{1}{\sqrt{C_L - C_L^2}} \hat{C}_{LR}\).

Next one can combine \(f^L_i\) and \(f^R_i\) to give wave functions for the unpartitioned system. One can show using the relations between the submatrices of \(\hat{C}\) that Eqn. (19) is an eigenstate of \(\hat{C}\) with eigenvalue 1, and hence is occupied. Now the eigenstates of \(\hat{C}_L\) and \(\hat{C}_R\) are the entanglement modes for the left and right sides of the systems. Hence \(F\) pairs up all the entanglement modes into occupied states. (There are two exceptions: if \(p_i = 0\) or 1, then \(\hat{M}\) is not well-defined. In the first case, \(f^R_i\) is definitely unoccupied, so there is no \(F_i\) corresponding to it. In the second case, \(f^R_i\) is definitely occupied and does not require a partner.)

The expression for the Schmidt weights has an intuitive relationship to the \(F\)'s. Since each \(F\) has its own electron with probability one, a term in the Schmidt decomposition is obtained (see Fig. [5b]) when a decision is made about which of these electrons are to reside on the right, say those in states \(F_j\) with \(j \in A_R\), and which are to reside on the left (those in states with \(j \in A_L\). The Schmidt coefficients \(\lambda_i^2\) are thus given by a Bernoulli distribution, \(\prod_{j \in A_R} p_i \prod_{j \in A_L} (1 - p_i)\), which is equivalent to Eq. (16). (Formally, one obtains this result by expanding \(|\Psi_G\rangle = \prod_{i,k_x} \left( \sqrt{p_i(k_\perp)} r^\dagger_{i,k_x} + \sqrt{1 - p_i(k_\perp)} \eta^\dagger_{i,k_x} \right) |0\rangle\).
Since $\hat{M}$ maps the right-half to the left half of the system, it can be combined with inversion symmetry, $\hat{I}$, to give the transformation used in Section VI, which transforms the entanglement spectrum of the right half into itself, $\mathcal{I}_S = \hat{I}\hat{M}$. Since it anticommutes with $\hat{C}_R - \frac{1}{2}$, $\hat{I}\hat{M}$ changes the sign of $p - \frac{1}{2}$ and hence of $e^i$, as well as the sign of $k_L$. It is also unitary. Thus, this transformation has the same properties as a two-dimensional “CRT” symmetry of the space parallel to the cut. Here $C$ is a particle-hole symmetry, $R$ is a 180° rotation and $T$ is time-reversal symmetry, although the system does not have those symmetries independently. The $C$ factor changes the sign of the energy, and all three factors change the sign of the momentum. The product of all three is unitary, like $\mathcal{I}_S$, because particle-hole symmetry is antiunitary when one considers how it acts on single-particle states.

This fact is enlightening since a CPT symmetry (with a reflection $P$ in place of rotation) could not be used to prove the masslessness of the Dirac excitations: any relativistic equation (including the massive Dirac equation) is invariant under CPT symmetry. (In two dimensions, inversion through the origin is not in place of rotation.)

### Appendix B: Parity of Finite Systems

The result that $(\hat{M}\hat{C})^2$ is a function only of the topological phase of an insulator (characterized by $\delta$) and of $k$, the number of excess particles in a Schmidt state, can be proved most easily by considering the inversion transformation of the ground state wave function of a finite system. This wave function must be an inversion eigenstate with some parity $(-1)^P$.

Notice by the way an important point that we have not discussed much: The products appearing in the Schmidt decomposition, Eq. (1), have to be antisymmetrized:

$$\langle \alpha R | \alpha L \rangle \equiv A.S. \{ \phi_{\alpha R} (r_1, r_2, \ldots, r_{N+1}) \} \tag{B1}$$

where “A.S.” means to antisymmetrize in all the variables. This wave function is not a product wave function, but it is the closest thing possible for Fermions: The correlations between densities on opposite sides of the cut vanish, surprisingly maybe.

Let us call the antisymmetrized-product wave function $\Phi_{\alpha}$. The inverse of this wave function is

$$\Phi_{\alpha} (-r_i) = A.S. \{ \Phi_{\alpha R} (-r_1, \ldots, -r_{N+1}) \Phi_{\alpha L} (r_{N+1} - r_1 + \ldots + r_i) \} \tag{B2}$$

The inversion of the factor corresponding to the right side of the system $\mathcal{I}\Phi_{\alpha R} = \Phi_{\alpha R} (-r_i)$ is a wave function on the left side. So we should compare this expression to $|\mathcal{I}\Phi_{\alpha L}| / |\Phi_{\alpha R}|$, which is equal to A.S. $\{ \Phi_{\alpha L} (-r_1, \ldots, -r_{N+1}) \Phi_{\alpha R} (-r_{N+1} - r_1 + \ldots + r_i) \}$. This differs from $\Phi_{\alpha} (-r_i)$ in the labelling of the coordinates. The parity of the permutation is $(-1)^{\frac{N-2}{2}} k$ and so

$$\mathcal{I}|\Phi_{\alpha R}| = (-1)^{\frac{N-2}{2}} |\mathcal{I}\Phi_{\alpha L}| / |\Phi_{\alpha R}| \tag{B3}$$

Now let us calculate the parity of the ground state of a noninteracting insulator by looking at a particular term in the Schmidt decomposition: Assume as we have been doing that there are $\delta$ pairs of zero energy states $\frac{1}{\sqrt{2}} (r_{ia}^l + r_{ib}^l)$ and $\frac{1}{\sqrt{2}} (r_{ia}^r + r_{ib}^r)$. Since each pair has the same parity $p$, $r_{ia,b} \leftrightarrow r_{ia,b}^\delta$. Then all the maximum weight states of the Schmidt decomposition are contained in $|M,W_\delta > = \prod_{i=1}^{\delta} (r_{2i-1} + r_{2i-1}^\delta + (r_{2i} + r_{2i}^\delta)) |S_R| |S_L|$. By Eq. (B3), the parity of $|S_R| |S_L|$ is $(-1)^{\frac{N-2}{2}}$. The product of all the Dirac mode operators is even under inversion, so the parity of $|M,W_\delta >$ is also $(-1)^{\frac{N-2}{2}}$. This also has to be the parity $(-1)^P$ of the entire ground state wave function, as was claimed in Section VII.

Now consider a generic term of the Schmidt decomposition of $|\Phi_G >$, such as $|\Phi_{\alpha} >$. Applying inversion to the Schmidt decomposition maps each term to another term except for a factor of $(-1)^P$. This is the case for $|\Phi_{\alpha} > = |\Phi_{\alpha R}| |\Phi_{\alpha L}|$, so $(-1)^P \cdot \hat{I} |\Phi_{\alpha R}| |\Phi_{\alpha L}|$ is another term in the Schmidt decomposition. Since $\hat{M}$ is defined to map each left-hand Schmidt state to its partner in the Schmidt decomposition, we can read off how $\hat{M}$ acts: it maps $|\Phi_{\alpha L}|$ to $|\Phi_{\alpha R}|$ and $|\Phi_{\alpha R}|$ to $(-1)^P \cdot \hat{I} |\Phi_{\alpha L}|$. Applying $(M\hat{C})^2$ to $|\Phi_{\alpha R}|$ therefore gives $(-1)^{P+k}$, for a state with $k$ extra Fermions on the right side.

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In fact, every entanglement eigenstate with a finite $e^\epsilon$ is a bound state of the surface, since the bulk dispersions are flat and equal to $\pm\infty$. States extend farther into the bulk as $|\epsilon|$ increases.

We need to assume that, if the model under consideration is a tight-binding model, then at least one center of inversion symmetry does not coincide with a site. Otherwise, there is no inversion-symmetric way of dividing the sites into two parts.

The relationship implies $I^* = e^{i\phi} I^{-1}$ (note, we can take the inverse since the determinant of $I$ is nonzero on account of the initial relationship). Now multiplying by $I$ on the left gives back $I \cdot I^* = 1 e^{i\phi}$. On the other hand, taking the complex conjugate of the original expression gives $I \cdot I^* = 1 e^{-i\phi}$ so $\phi = 0, \pi$.

One could send the crystal toward a beam-splitting “mirror” which inverts the crystal with probability one-half, and then interfere the beams. Making a mirror that can turn the crystal inside-out like this is even harder than “just” maintaining the coherence of a macroscopic crystal during an interference experiment!

Whether the two sides of the system are correlated or not on this wave function depends on whether one is looking at an “Eulerian representation,” (as it is called in the context of fluid mechanics) with variables that are localized in space (such as particle number) or a “Lagrangian representation,” with variables that are attached to specific particles (their positions, for example). In the Lagrangian representation, the variables $r_1$ and $r_2$ are entangled.