Many-body generalization of the $Z_2$ topological invariant for the quantum spin Hall effect

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We propose a many-body generalization of the $Z_2$ topological invariant for the quantum spin Hall insulator, which does not rely on single-particle band structures. The invariant is derived as a topological obstruction that distinguishes topologically distinct many-body ground states on a torus. It is also expressed as a Wilson-loop of the SU(2) Berry gauge field, which is quantized due to time-reversal symmetry.

A topological insulator is a quantum phase of matter with a bulk energy gap that cannot be deformed continuously to a trivial band insulator without going through a quantum phase transition. The most prominent example is the quantum Hall (QH) state. For instance, the Kane-Mele model generalized by adding interactions.

The QH states are characterized by a topological order in the bulk is also robust against weak interactions. It is the purpose of this paper to construct a many-body generalization of the $Z_2$ topological invariant that detects such bulk $Z_2$ topology. When interactions are weak, the construction of the $Z_2$ topological order in the bulk is also robust against those perturbations. It is the purpose of this paper to construct a many-body generalization of the $Z_2$ topological invariant that detects such bulk $Z_2$ topology. When interactions are weak, the construction of the $Z_2$ topological order in the bulk is also robust against those perturbations.

Topological orders in QH states are associated with the charge degrees of freedom of electrons and accompanied by broken time-reversal symmetry (TRS). Recently, Kane and Mele have established a topological classification in time-reversal (TR) invariant noninteracting systems associated with the spin degrees of freedom. Considering the doubled version of the Haldane model for the integer QH effect as an example, they showed that there exists a new type of topological insulators, quantum spin Hall (QSH) insulators, which are characterized by an odd number of Kramers pairs of gapless edge modes. In contrast, trivial insulators have an even number of pairs. QSH insulators in the bulk are characterized by a $Z_2$ number.

Although the QSH insulator has been proposed in a noninteracting system, the even or odd parity in the number of Kramers pairs of edge modes is robust against weak interactions that respect TRS. This suggests that the $Z_2$ topological order in the bulk is also robust against those perturbations. It is the purpose of this paper to construct a many-body generalization of the $Z_2$ invariant that detects such bulk $Z_2$ topology. When interactions are weak, the construction of the $Z_2$ invariant might not be unique, and hence the corresponding strongly interacting many-body state can be characterized by a multiplet of $Z_2$ invariants.

We put a many-body system with a fixed number of particles on a 2D torus $T^2$ with $N = L_x \times L_y$ unit cells, each of which has $m$ sites, where $N$ is assumed to be odd. We focus on the case with $m = 2$ which includes the Kane-Mele model generalized by adding interactions. Consider a deformation of the Hamiltonian by threading magnetic fluxes $0 \leq \alpha_{x,y} \leq 2\pi$ through the two cycles of the torus where $\alpha_x (\alpha_y)$ denotes the flux threaded along the $x(y)$ directions. The space of the Hamiltonian $H_0$ obtained by the flux-threading.

![FIG. 1: (a) The torus in real space where magnetic fluxes $\alpha_{x,y}$ are threaded in the $x,y$-cycles, respectively. (b) The space of the Hamiltonian $H_0$ obtained by the flux-threading. The doublet $\nu^A(\alpha)$ (or $\nu^B(\alpha)$) is well-defined in the patch A(B).](image)

The QSH states are characterized by a topological obstruction of the $U(1)$ bundle on $T^2_0$, i.e., inability to smoothly define the ground state over $T^2_0$, which is signaled by a $U(1)$ Chern number. On the other hand, in the QSH effect, the $U(1)$ Chern number always vanishes because of TRS. Therefore, there exists a unique $2N$-particle ground state with a finite energy gap at each point $\alpha \in T^2_0$.

Using the quasiparticle Green’s function, we consider the following many-electron states obtained by creating $N$ holes in the ground state,

$$|t, s(\alpha)\rangle = \left(\prod_{r=1}^N c_{r,t,s}\right)|\Psi^0\rangle,$$  \quad (1)
where \( c^+_{r,t,s}/c_{r,t,s} \) creates/annihilates an electron with spin \( s \uparrow, \downarrow \) at a site \( t = 1, 2 \) within a unit cell labeled by \( r \). If \( d(\alpha):= \det(1,s[1,s') \neq 0 \), the vector space spanned by the states \( |1, \uparrow(\alpha)\rangle \) and \( |1, \downarrow(\alpha)\rangle \) is two-dimensional, and a doublet of orthonormal states \( \langle v(\alpha)|2(\alpha)\rangle \) can be obtained from suitable linear combinations, \( (n(\alpha)) = \sum_{s=\uparrow, \downarrow} u_{n,s}(\alpha)|1,s(\alpha)\rangle \) with \( n = 1, 2 \). \( u_{n,s}(\alpha) \) is chosen so that \( (n(\alpha)|A_{n,m}(\alpha) = \delta_{n,m} \). From the doublet, we can define a projection operator \( P(\alpha) = |1(\alpha)\rangle\langle 1(\alpha)| + |2(\alpha)\rangle\langle 2(\alpha)| \).

In the case of non-interacting electrons (such as the Kane-Mele model), the doublet \( v(\alpha) \) can be constructed from the Bloch wavefunctions, and the specific way of creating the doublet, e.g., choice of the sublattice we made \((t = 1)\) at which we remove electrons, does not matter, i.e., different choices of sublattice lead to the same projection operator. When we perturb the system by weak interactions, since \( d(\alpha) \) cannot vanish abruptly, the above construction of the doublet \( v(\alpha) \) smoothly interpolates non-interacting and interacting cases. However, in general, \( d(\alpha) \) can vanish at some points in \( T_{\alpha}^2 \) where the two states \( |1,s(\alpha)\rangle \) with \( s = \uparrow, \downarrow \) fail to span a 2D vector space. Since \( d(\alpha) \) is a real function defined on the 2D space \( T_{\alpha}^2 \), \( d(\alpha) \) can vanish either on lines or points in \( T_{\alpha}^2 \). \( d(\alpha) \) cannot vanish on a 2D submanifold of \( T_{\alpha}^2 \) unless \( d(\alpha) \) is identically zero since the ground state \( \langle \Psi^\alpha \rangle \), and hence \( d(\alpha) \) as well, are analytic on \( T_{\alpha}^2 \). If \( d(\alpha) \) vanishes at all points in \( T_{\alpha}^2 \), we can perturb our Hamiltonian slightly without closing the gap so that \( d(\alpha) \) becomes nonzero everywhere except for some lines and points. Since the dimension of the submanifold where \( d(\alpha) \) vanishes is smaller than 2, we can analyticaly continue the 2D projection operator \( P(\alpha) \) to the whole \( T_{\alpha}^2 \) generically. One may think that such a smooth continuation may not work because there can be points \( \alpha_i \) at which one (or a linear combination) of the doublet \( |1,s(\alpha)\rangle \) vanishes either due to a scalar vortex (winding in the phase of the coefficient of a quantum state with a vanishing norm at the center), i.e., \( |1,s(\alpha)\rangle = (a_{\alpha} - a_{\alpha i}|\psi_1\rangle + i(a_{\alpha} - a_{\alpha i})|\psi_2\rangle \) or due to a vector vortex (winding between two quantum states with a vanishing norm at the center), i.e., \( |1,s(\alpha)\rangle = (a_{\alpha} - a_{\alpha i})|\psi_1\rangle + (a_{\alpha} - a_{\alpha i})|\psi_2\rangle \) where \( |\psi_1\rangle \) and \( |\psi_{\alpha i}\rangle \) are well-defined states with \( \langle \psi_1|\psi_{\alpha i}\rangle = 0 \). For scalar vortices, \( P(\alpha) \) can be smoothly extended because the projection operator is insensitive to the overall phase. On the other hand, for vector vortices \( P(\alpha) \) cannot be smoothly defined. However, one can generically avoid the occurrence of the latter points by adding a small TR symmetric perturbation to the Hamiltonian. If we add a perturbation, the points where the norm vanishes will disappear because the state will generically change as \( |1,s(\alpha)\rangle \rightarrow |1,s(\alpha)\rangle + A(\alpha)|\psi_i^s\rangle \) where \( A(\alpha) \neq 0 \) at \( \alpha = \alpha_i \) and \( |\psi_i^s\rangle \) is generically independent with \( |\psi_{\alpha i}\rangle \) and \( |1,s(\alpha)\rangle \). In this way, the 2D projection operator \( P(\alpha) \) can be smoothly defined in the whole \( T_{\alpha}^2 \).

We now choose \( v(\alpha) \) such that it satisfies the TRS condition, \( v(-\alpha)(i\sigma_2) = \Theta v(\alpha) \), where \( \Theta \) is the TR operator \[13\]. Note that when acting on \( v(\alpha) \), which consists of \( N \)-electron states, \( \Theta^2 = -1 \). While this is always possible locally since \( \Theta P(\alpha)\Theta^{-1} = P(-\alpha) \), there is no guarantee that such basis can be defined globally. Therefore, we first divide \( T_{\alpha}^2 \) into two patches (\( A \) and \( B \)) as shown in Fig. \[1\] (b), and see whether we can merge them into a single patch or not. In each patch, we have a doublet \( v^p(\alpha) = (|1^p(\alpha)\rangle,|2^p(\alpha)\rangle) \) \( (p = A,B) \), satisfying \( (n^p(\alpha)|m^p(\alpha) = \delta_{n,m}, v^p(-\alpha)|\sigma_2 = \Theta v^p(\alpha) \), and \( P(\alpha) = (|1^p(\alpha)\rangle(|1^p(\alpha)\rangle + |2^p(\alpha)\rangle\langle 2^p(\alpha)|) \).

![FIG. 2: Two topologically different paths the SU(2) matrix \( g(\alpha) \) can take as the angle \( \varphi \) in \( A \cap B \) changes from 0 to \( \pi \).

The path in (a) is contractible while the path in (b) is not because \( g(-\alpha) \) should be at the opposite point of the \( g(\alpha) \) in \( S^3 \). Since \( v^A(\alpha) \) and \( v^B(\alpha) \) span the same 2D Hilbert space at \( \alpha \in A \cap B \), they are related by \( v^A(\alpha) = v^B(\alpha)M(\alpha) \), where \( M(\alpha) \) is a U(2) matrix (transition function). Using the TRS condition, we obtain a relation between the transition function at \( -\alpha \) and \( \alpha \), \( M(-\alpha) = \sigma_2 M^*(\alpha)\sigma_2 \). If we decompose \( M(\alpha) \) into a U(1) phase \( \theta(\alpha) \) and an SU(2) matrix \( g(\alpha) \), we have the two possibilities,

\[
\begin{align*}
& a) \quad \theta(-\alpha) = -\theta(\alpha) \quad \text{and} \quad g(-\alpha) = g(\alpha), \\
& b) \quad \theta(-\alpha) = -\theta(\alpha) + \pi \quad \text{and} \quad g(-\alpha) = -g(\alpha). \quad (2)
\end{align*}
\]

In the TR invariant system, the U(1) phase cannot have a non-trivial winding. However, the SU(2) matrix has two topologically distinctive configurations. In the case a), we can deform a ground state continuously such that the trajectory of \( g(\alpha) \) as a function of \( \varphi \), where \( \varphi \) parameterizes the overlapping region \( A \cap B \) which has the topology of \( S^1 \), is contractable to a point in the space of SU(2) matrices as shown in Fig. 2 (a). On the other hand, in the case b), the trajectory of \( g(\alpha) \) is not contractible because \( g(-\alpha) = -g(\alpha) \) as shown in Fig. 2 (b). Therefore, a state in the class b) cannot be continuously deformed to a state in class a). The relative sign between \( g(\alpha) \) and \( g(-\alpha) \) is the \( Z_2 \) topological invariant. If there is no interaction, \( \alpha \) plays the role of momenta of Bloch states and the topological invariant reduces to the existing \( Z_2 \) invariant \[2\]. In the present scheme, the \( Z_2 \) invariant can be generalized to interacting cases. Since the generalized \( Z_2 \) invariant is quantized, it cannot change abruptly upon turning on interactions.

Then when can the \( Z_2 \) invariant change, as we tune some parameters (other than \( \alpha \)) of the Hamiltonian,
The condition that sews local frames at $\alpha$ and $-\alpha$ together naturally induces a constraint on the Berry gauge field configuration,

$$A_\mu(-\alpha) = w(\alpha)A_\mu^T(\alpha)w^\dagger(\alpha) - w(\alpha)\partial_\mu w^\dagger(\alpha). \quad (3)$$

Accordingly, the U(1) and SU(2) gauge fields are constrained as $a_\mu^0(-\alpha) = a_\mu^0(\alpha) - 2\partial_\mu \zeta(\alpha)$, and $a_\mu(-\alpha) \cdot \sigma/(2i) = a_\mu(\alpha) \cdot \tilde{w}(\alpha)\sigma^T\tilde{w}(\alpha)/(2i) - \tilde{w}(\alpha)\partial_\mu \tilde{w}(\alpha)$, where we decomposed $\tilde{w}(\alpha)$ into the U(1) ($e^{i\epsilon}$) and SU(2) ($\tilde{w}$) parts, $w(\alpha) = e^{i\epsilon}(\alpha)\tilde{w}(\alpha)$. (Note that this decomposition has a global sign ambiguity, which will not affect the following discussions.) At the TR symmetric points, $\tilde{w}(\alpha)$ is equal to $i\sigma_2$ up to sign, $\tilde{w}(\alpha) = \text{Pf}[\tilde{w}(\alpha)] \times i\sigma_2$, where Pf $[\tilde{w}]$ is the Pfaffian of $\tilde{w}$.

![FIG. 3: Four time-reversal invariant loops $C_{1,2,3,4}$ on $T_\alpha^2$, and a loop $\partial(T_\alpha^2/2)$ that encloses the half of $T_\alpha^2$.](image)

Following Ref. [1] a natural object to consider, which is invariant under $\alpha$-dependent U(2) transformations of the local frame, is an SU(2) Wilson loop

$$W[C] = \frac{1}{2} \text{Tr} \left\{ P \exp \left[ \int_C d\alpha^\mu a_\mu(\alpha) \cdot \frac{\sigma}{2i} \right] \right\}, \quad (4)$$

where $P$ represents the path ordering and $C$ is a closed loop on the $\alpha$ plane. An essential observation is that for loops $C$ that are invariant under TRS (i.e., loops that are mapped onto themselves by TRS up to orientation), the sewing condition [3] quantizes the SU(2) Wilson loops, $W[C] = \pm 1$. For example, for a straight loop $C_1$ running from $(-\pi, 0)$ to $(\pi, 0)$ (Fig. [3]), $W[C_1] = \text{Pf}[\tilde{w}(\pi, 0)] \text{Pf}[\tilde{w}(0, 0)]$.

Although being invariant under a gauge transformation induced by a unitary transformation of the local frame at $\alpha$, each Wilson loop is not invariant under redefinition of unit cells. For example, when there are only two orbitals ($t = 1, 2$) in each unit cell, a spin-dependent redefinition of unit cell $c_{r,1,s} \rightarrow c_{r,1,s} - c_{r+spx,2,s}$, $p \in Z$ flips the sign of $W[C_1]$ and $W[C_2]$ when $p$ is odd, where $x$ is a unit lattice translation vector in $x$ direction. In other word, this transformation inserts a half unit of
the SU(2) flux along the \(\alpha_x\)-direction. When there is translation invariance, the choice of unit cells is arbitrary, whereas if we introduce a boundary, the choice of unit cell should be consistent with the location of the boundary. In this sense, the (quantized) value of each Wilson loop matters when we terminate the system.

We can construct, however, from two parallel Wilson loops (e.g., \(C_1\) and \(C_2\)), an invariant which is left unchanged by the half-flux insertion in \(\alpha_x\) and \(\alpha_y\) directions, since the effect of the half-flux insertion cancels. We are thus led to consider a Wilson loop that runs counterclockwise around the boundary of the half of \(T_\alpha^2\), \(T_\alpha^2/2 := (-\pi, \pi) \times [0, \pi]\), say (Fig. 3):

\[
W[\partial(T_\alpha^2/2)] := (-1)^\Delta = \prod_{k=(0,0),(\pi,0), (\pi,\pi), (0,\pi)} \text{Pf} [\hat{w}(k)].
\] (5)

The \(Z_2\) number \(\Delta\) distinguishes trivial (\(\Delta = 0\)) and non-trivial (\(\Delta = 1\)) insulators. The Kane and Mele model\[7\] is an explicit example of the latter case.

The connection between the gluing and the gauge pictures can be established for the non-interacting case with conserved \(S^z\). In this case, the ground state can be written as \(|\Psi_\alpha\rangle = |\Psi_\alpha^1\rangle \times |\Psi_\alpha^2\rangle\) and the doublet becomes \(v(\alpha) = (|\Psi_\alpha^1\rangle, |\Psi_\alpha^2\rangle)\). The \(Z_2\) invariant obtained in the gluing picture is nothing but \((-1)^{\text{Ch}_1} = (-1)^{\text{Ch}_1}\). On the other hand, the quantized SU(2) Wilson loop also gives \(W[\partial(T_\alpha^2/2)] = (-1)^{\text{Ch}_1}\). The \(Z_2\) invariant is independent of the choice of sublattice in Eq. \[14\] because annihilating \(N\) electrons of spin \(s\) results in the same state of \(|\Psi_\alpha^s\rangle\) irrespective of the choice of sublattice. Since the quantized \(Z_2\) number cannot change abruptly as we turn on interactions or disorders, it is the only topological invariant in weakly interacting TRS systems. Thus the \(Z_2\) invariant is a natural generalization of the parity (even/odd) of the Chern number, to the case without the \(S^z\) conservation in which case the Chern number cannot be defined.

Finally, a few remarks are in order. First, if we add some perturbations which enlarge the size of the unit cell from \(m = 2\) to \(m > 2\), we can still remove half of the total electrons at the original location to calculate the \(Z_2\) invariant. This allows one to characterize the topological order of systems which have both interactions and disorder\[12\]. Second, the formalism developed so far can be extended to three dimensions similarly\[14, 19, 20\].

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