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Time Reversal Polarization and a Z_2 Adiabatic Spin Pump

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Abstract

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Time reversal polarization and a Z_2 adiabatic spin pump

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We introduce and analyze a class of one-dimensional insulating Hamiltonians that, when adiabatically varied in an appropriate closed cycle, define a "Z_2 pump." For an isolated system, a single closed cycle of the pump changes the expectation value of the spin at each end even when spin-orbit interactions violate the conservation of spin. A second cycle, however, returns the system to its original state. When coupled to leads, we show that the Z_2 pump functions as a spin pump in a sense that we define, and transmits a finite, though nonquantized, spin in each cycle. We show that the Z_2 pump is characterized by a Z_2 topological invariant that is analogous to the Chern invariant that characterizes a topological charge pump. The Z_2 pump is closely related to the quantum spin Hall effect, which is characterized by a related Z_2 invariant. This work presents an alternative formulation that clarifies both the physical and mathematical meaning of that invariant. A crucial role is played by time reversal symmetry, and we introduce the concept of the time reversal polarization, which characterizes time reversal invariant Hamiltonians and signals the presence or absence of Kramers degenerate end states. For noninteracting electrons, we derive a formula for the time reversal polarization that is analogous to Berry's phase formulation of the charge polarization. For interacting electrons, we show that Abelian bosonization provides a simple formulation of the time reversal polarization. We discuss implications for the quantum spin Hall effect, and argue in particular that the Z_2 classification of the quantum spin Hall effect is valid in the presence of electron electron interactions.

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I. INTRODUCTION

In recent years, the advent of spintronics has motivated the search for methods of generating spin currents with little or no dissipation. One class of proposals involves designing an adiabatic pump in which the cyclic variation of some control parameters results in the transfer of spin across an otherwise insulating structure.[1–4] Such a spin pump has been realized in quantum dot structures.[5] A second class of proposals involves using the spin Hall effect to generate a spin current using an electric field.[6,7] Interest in this approach has been stimulated by the experimental observation of spin accumulation induced by the spin Hall effect in doped GaAs structures.[8,9] In these experiments, the spin current is accompanied by a dissipative charge current. This motivated Murakami, Nagaosa, and Zhang[10] to propose an interesting class of "spin Hall insulator" materials, which are band insulators that have, according to a Kubo formula, a large spin Hall conductivity. However, the spin current that flows in the bulk of these materials is not a transport current, and cannot be simply measured or extracted. A crucial ingredient for the generation of transport currents is the existence of gapless extended edge states. Such states are generically not present in the spin Hall insulators.[11]

Motivated by the spin Hall insulator proposal, we introduced a model of graphene in which the symmetry allowed spin-orbit interactions lead to a quantum spin Hall effect.[12,13] A related phase has been proposed for GaAs in the presence of a uniform strain gradient.[14] This phase is characterized by a bulk excitation gap and gapless edge excitations. In the special case where the spin S_z is conserved, this phase can be viewed as two copies of the quantum Hall state introduced by Haldane.[15] The phase persists, however, in the presence of spin nonconserving interactions as well as disorder.[12,13,16] Time reversal symmetry protects the gapless edge states when electron interactions are weak, though strong interactions can open an energy gap at the edge accompanied by time reversal symmetry breaking.[17,18] We argued that the quantum spin Hall phase is distinguished from a band insulator by a Z_2 topological index,[13] which is a property of the bulk system defined on a torus. We suggested a formula for this index in terms of the Bloch wave functions. However, the physical meaning of this formula and its relation to the edge states was not explicit.

When placed on a cylinder (or equivalently a Corbino disk), the quantum spin Hall system defines a kind of adiabatic pump as a function of the magnetic flux threading the cylinder. In the case in which S_z is conserved, advancing the flux by one flux quantum results in the transfer of spin $\Delta S_z = \hbar$ from one end of the cylinder to the other. This is a spin pump, whose operation is analogous to a charge pump that could be constructed with a quantum Hall state on a cylinder. As envisioned by Thouless and co-workers in the 1980s,[19,20] the adiabatic charge pumping process is characterized by a topological invariant—the Chern number—which is an integer that determines the quantized charge that is pumped in the course of a cycle. Equivalently, the Chern number provides a topological classification of the two-dimensional quantum Hall state.[21–24] When S_z is conserved, similar ideas can be used to describe a quantized adiabatic spin pump.[4]

A local conservation law is essential for this type of topological pumping process. For a finite system with closed ends, the eigenstates before and after a complete cycle must be distinct. This means that two energy levels must cross in the course of the cycle. In the case of the charge pump, that level crossing is protected by local charge conservation because the two states differ in their eigenvalue of the charge at each end. In the absence of a conservation law there will, in general, be no level crossings, and the system will be in the same state before and after the cycle.

Unlike charge, spin does not obey a fundamental conservation law, so unless spin nonconserving processes can be made very small, it is not possible to define an adiabatic spin pump that works analogously to the Thouless charge pump. Nonetheless, in Ref. 13 we argued that *time reversal symmetry* introduces a conservation law that allows for a topological pumping process. Specifically, we showed that for a quantum spin Hall state on a cylinder, the eigenstates before and after adiabatic flux insertion are orthogonal, and cannot be connected by any local time reversal invariant operator. When a second flux is added, however, the system returns to its original ground state. In this sense, the quantum spin Hall effect defines a "Z_2 pump." In one cycle, there is no charge transferred between the two ends. Since spin is not conserved, the two states cannot be distinguished by a spin quantum number (though the expectation value of the spin at the end changes by a nonquantized amount). The following question therefore arises: What is it that is pumped between the ends of the cylinder?

In this paper, we examine this issue carefully and introduce a class of one-dimensional models that exhibit a similar pumping behavior that is protected by time reversal symmetry. The "Z_2 spin pump" is analogous to the quantum spin Hall effect in the same sense that the charge pump is analogous to the ordinary quantum Hall effect. We introduce the concept of the *time reversal polarization*, a Z_2 quantity that signals whether a time reversal invariant one-dimensional system has a Kramers degeneracy associated with its ends. We show that the change in the time reversal polarization in the course of an adiabatic cycle is related to a Z_2 topological invariant that distinguishes a Z_2 spin pump from a trivial cycle of an insulator that pumps nothing. This Z_2 invariant is equivalent to the invariant introduced in Ref. 13 to characterize the quantum spin Hall effect. The present work, however, provides an alternative formulation that clarifies both the physical and mathematical meaning of the invariant.

We study a family of one-dimensional Hamiltonians that have a bulk energy gap and a length that is much larger than the exponential attenuation length associated with that gap. We suppose the Hamiltonian depends continuously on a "pumping parameter" t, satisfying the following properties:

$$H[t+T]=H[t], \tag{1.1}$$

$$H[-t]=\Theta H[t]\Theta^{-1}, \tag{1.2}$$

where Θ is the time reversal operator. t should be viewed as a variable that parametrizes the instantaneous Hamiltonians in an adiabatic cycle. In order for t to be interpreted as the physical time, the adiabatic condition $dH/dt \ll H\Delta E/\hbar$ must be satisfied, where ΔE is a characteristic energy gap.

In the case in which the one-dimensional system corresponds to a two-dimensional system on a cylinder, t/T may be viewed as the magnetic flux threading the cylinder in units of the flux quantum. In the course of the cycle, time reversal symmetry is broken. However, the second constraint ensures that the system passes through *two* distinct points $t_1^*=0$ and $t_2^*=T/2$ at which the Hamiltonian is time reversal invariant. Condition (1.2) may be relaxed somewhat, but it is essential that there exist two distinct time reversal invariant points t_1^* and t_2^* where Eq. (1.2) is locally valid. The existence of two such points plays a crucial role in the topological classification of the pumping cycle. In particular, we will show that pumping cycles in which $H[t_1^*]$ and $H[t_2^*]$ have different time reversal polarization are topologically distinct from trivial cycles.

We will begin in Sec. II by introducing a simple one-dimensional tight-binding model that exemplifies the Z_2 spin pump. This model is closely related to a model of a spin pump that was recently introduced by Shindou[4], which may be applicable to certain spin-$\frac{1}{2}$ quantum spin chains, such as Cu-benzoate and Yb_4As_3. This tight-binding model incorporates spin nonconserving spin-orbit interactions and provides a concrete illustration of the Z_2 pumping effect.

In Sec. III, we provide a general formulation of the time reversal polarization for noninteracting electrons. Our discussion closely parallels the theory of charge polarization,[25–29] in which the charge polarization is related to Berry's phase of Bloch wave functions. We show how the change in the time reversal polarization defines a Z_2 topological invariant characterizing the pumping cycle.

In Sec. IV, we argue that the notion of time reversal polarization and the topological classification that follows from it can be generalized to interacting systems. We describe an interacting version of our 1D model using Abelian bosonization. This provides a different formulation of the time reversal polarization, which is well defined in the presence of interactions.

In Sec. V, we conclude by addressing two issues. In Sec. V A, we discuss the implications of the time reversal polarization for the quantum spin Hall effect. We argue that the two-dimensional quantum spin Hall phase is a distinct phase from a band insulator even in the presence of electron electron interactions. We then prove that this phase either has gapless edge excitations or exhibits a ground-state degeneracy associated with time reversal symmetry breaking at the edge. We also comment on a proposal by Sheng, Weng, Sheng, and Haldane[30] to classify the quantum spin Hall effect in terms of a Chern number matrix.

In Sec. V B, we ask whether the Z_2 spin pump we have defined can actually pump spin. Despite the fact that the isolated pump returns to its original state after two cycles, we argue that when connected weakly to leads, the Z_2 pump *does* pump spin, although the amount of spin pumped in each cycle is not quantized.

In the Appendix, we relate different mathematical formulations of the Z_2 topological invariant. We begin by showing that, like the Chern invariant, the Z_2 invariant can be interpreted as an obstruction to globally defining wave functions, *provided* a constraint relating time reversed wave functions is enforced. We then prove that the invariant derived in this paper is equivalent to the one introduced in Ref. 13.

II. TIGHT-BINDING MODEL

In this section, we introduce a one-dimensional tight-binding model of the Z_2 spin pump. This model is closely related to a model introduced by Shindou as an adiabatic spin pump.[4] Shindou considered an antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain to which two perturbations that open a gap in the excitation spectrum are added. The first term is a stag-

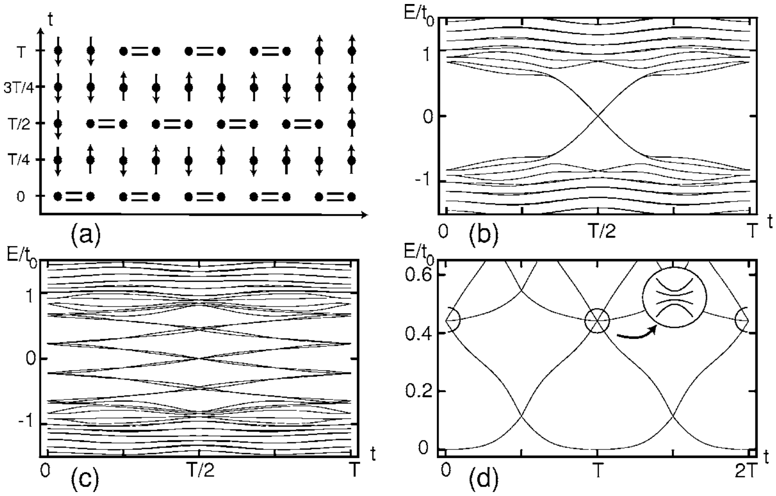

FIG. 1. (a) Schematic representation of the ground state of Eqs. (2.1)–(2.5) for various values of the pumping parameter t. The ground states at the time reversal invariant points $t=0$ and $t=T/2$ are distinguished by the presence of Kramers degenerate end states. (b) Single-particle energy levels $E_n(t)$ for a 24-site chain with $\Delta t_{\rm st}^0/t_0=0.4$, $h_{\rm st}^0/t_0=0.8$, and $\vec{e}_{\rm so}/t_0=0.1\hat{y}$. (c) Single-particle energy levels $E_n(t)$ for a 24-site chain with 12 extra sites added at each end. (d) Low-energy many-body energy levels associated with one end of the chain. The degeneracy at $t=T/2$ and $t=3T/2$ is protected by time reversal symmetry. The inset shows how electron electron interactions lift the degeneracy at $t=0$, T, and $2T$.

gered magnetic field $h_{\rm st}$ that locks the spins into a Neel ordered state. The second is a staggered component to the exchange interaction $\Delta J_{\rm st}$, which leads to a dimerized state. Interestingly, Shindou suggested that this model may be relevant to certain $S=\frac{1}{2}$ quantum spin chains, such as Cu-benzoate and Yb_4As_3, in which spins reside at two crystallographically inequivalent sites. He argued that in these systems $h_{\rm st}$ can be controlled by applying a *uniform* magnetic field, and $\Delta J_{\rm st}$ can be controlled with a uniform electric field.

Shindou showed that a cycle in which $\Delta J_{\rm st}$ and $h_{\rm st}$ are adiabatically varied defines a topological spin pump, which transfers $S_z=\hbar$ in each cycle. The topological quantization of Shindou's pump requires the conservation of S_z. In general, however, S_z nonconserving processes are allowed by symmetry. In particular, the Dzyaloshinskii-Moriya interaction, $\mathbf{d}\cdot(\mathbf{S}_1\times\mathbf{S}_2)$, is allowed, and will inevitably lead to the violation of S_z conservation. We will argue, however, that provided the system retains time reversal invariance when $h_{\rm st}=0$, this system remains a Z_2 spin pump even in the presence of the Dzyaloshinskii-Moriya interaction.

We study a noninteracting electron version of the Shindou model, where in addition to the spin degree of freedom we allow charge fluctuations. Consider a one-dimensional tight-binding model with a staggered magnetic field, a staggered bond modulation, as well as a time reversal invariant spin orbit interaction,

$$H = H_0 + V_h + V_t + V_{\rm so}, \tag{2.1}$$

where

$$H_0 = t_0 \sum_{i,\alpha} (c_{i\alpha}^\dagger c_{i+1\alpha} + c_{i+1\alpha}^\dagger c_{i\alpha}), \tag{2.2}$$

$$V_h = h_{\rm st} \sum_{i,\alpha\beta} (-1)^i \sigma_{\alpha\beta}^z c_{i\alpha}^\dagger c_{i\beta}, \tag{2.3}$$

$$V_t = \Delta t_{\rm st} \sum_{i,\alpha} (-1)^i (c_{i\alpha}^\dagger c_{i+1\alpha} + c_{i+1\alpha}^\dagger c_{i\alpha}), \tag{2.4}$$

and

$$V_{\rm so} = \sum_{i,\alpha,\beta} i\vec{e}_{\rm so}\cdot\vec{\sigma}_{\alpha\beta}(c_{i\alpha}^\dagger c_{i+1\beta} - c_{i+1\alpha}^\dagger c_{i\beta}). \tag{2.5}$$

Here $\vec{e}_{\rm so}$ is an arbitrary vector characterizing the spin-orbit interaction. This term explicitly violates the conservation of S_z, playing a role similar to the Dzyaloshinskii-Moriya interaction in Shindou's model. We consider an adiabatic cycle in which

$$(\Delta t_{\rm st}, h_{\rm st}) = (\Delta t_{\rm st}^0 \cos(2\pi t/T), h_{\rm st}^0 \sin(2\pi t/T)). \tag{2.6}$$

For $\vec{e}_{\rm so}=0$, the energy gap is $\Delta E=\sqrt{h_{\rm st}^2+4\Delta t_{\rm st}^2}$, so the adiabatic condition is satisfied for $T \gg \hbar/\min(h_{\rm st}^0, 2\Delta t_{\rm st}^0)$. Since V_h is odd under time reversal, while V_t is even, condition (1.2) is clearly satisfied. At $t=0$ and $T/2$, the Hamiltonian is time reversal invariant.

In Fig. 1(a), we depict ground states in the strong-coupling limit at representative points along the adiabatic cycle. At $t=T/4$ and $3T/4$, V_h dominates and locks the spins into a Neel ordered state. At $t=0$ and $T/2$, V_t dominates, and the system is dimerized with singlet pairs of electrons occupying alternate bonds. Importantly, the ground state at $t=T/2$ is distinguished from the ground state at $t=0$ by the presence of *unpaired* spins at each end.

When $V_{\rm so}=0$, S_z is conserved, and this model describes a spin pump. In this case, V_h+V_t can be decomposed into two independent periodic potentials that lock the densities of the up and down spin particles and slide in opposite directions as a function of t. As t evolves from 0 to T, the periodic potentials slide by one lattice constant. Provided there is "space" for the added spin at the ends, spin $\hbar$ will accumulate at the end following each cycle.

We wish to understand how this spin pump is modified when $V_{\rm so}\neq 0$, so that S_z is not conserved. In Fig. 1(b), we plot the single-particle energy levels for a 24-site chain as a function of t for nonzero $V_{\rm so}$. The bulk energy gap can be clearly seen with continuum states above and below. The energy levels that cross the gap are end states. Each line consists of two states that are localized at opposite ends. The crossing of the end states at $t=T/2$ will play a critical role in what follows. When $V_{\rm so}=0$, the degeneracy at $T/2$ is protected by spin conservation because the two states at each edge have $S_z = \pm\hbar/2$. Nonzero V_{so} does *not* lift the degeneracy provided the Hamiltonian remains time reversal invariant at $T/2$. The two end states form a Kramers doublet whose degeneracy cannot be broken by any time reversal invariant perturbation.

Because of the level crossing at $t=T/2$ it is clear that a system that starts in the ground state at $t=0$ will be in an excited state at $t=T$. However, since the end states merge with the continuum, the excitation will not be localized near the edge, and bulk particle-hole pairs will be excited. This is because there is no "space" to put the excitations at the ends. In Sec. V B, we will discuss the effect of connecting this pump to reservoirs that allow the end states to be "emptied" without exciting bulk particle-hole pairs. For the purpose of this section, however, we will study the operation of an isolated pump by adding several sites at the ends of the chain for which V_h and V_t vanish. This introduces additional midgap states localized at each end, allowing the cycle to proceed without generating bulk excitations.

Figure 1(c) shows the energy levels as a function of t with the extra sites added at each end. There are now several midgap states at each end. Since all of the midgap states are localized at one end or the other, the low-energy excitations of the system can be factorized as a product of excitations at each of the two ends.

In Fig. 1(d), we plot for $0<t<2T$ the energies of the lowest few many-body eigenstates associated with a single end, obtained by considering particle-hole excitations built from the single-particle states localized at that end. Though this picture was computed for noninteracting electrons, it is clear that the Kramers degeneracy of the ground state at $t=T/2$ and $3T/2$ will be robust to the addition of electron-electron interactions. The first excited state at $T=0$, T, and $2T$ in Fig. 1(d) is fourfold degenerate (the middle level coming into that point is doubly degenerate). This degeneracy, however, is an artifact of noninteracting electrons. The degeneracy is present because there are four ways of making particle-hole excitations with two pairs of Kramers degenerate states. Electron-electron interactions, however, will in general split this degeneracy, as shown in the inset, so there will be no level crossing at $t=T$.

We thus conclude that when the isolated pump starts in its ground state at $t=0$, it arrives in an excited state after one complete cycle at $t=T$. After a second cycle, however, at $t=2T$ the system returns to its original state. For this reason, we call it a "Z_2 pump." It is possible that by coupling to other degrees of freedom, an *inelastic* process (such as emitting a phonon) could cause the excited state to relax back to the ground state. Nonetheless, there is an important distinction between this adiabatic process that generates an excited state and one that does not. In Sec. V B, we will return to this issue when we discuss connecting the pump to leads. The nontrivial operation of a single cycle depends critically on the time reversal symmetry at $t=T/2$. Breaking time reversal symmetry at that point leads to an avoided crossing of the energy levels, so that the system returns adiabatically to its original state at $t=T$.

From the point of view of the end states, the nontrivial pumping effect arises because there exist Kramers degenerate end states at $t=T/2$, but not at $T=0$. In the next section, we show that this property is determined by the topological structure of the *bulk* Hamiltonian, $H(t)$.

III. TIME REVERSAL POLARIZATION AND Z_2 INVARIANT

In this section, we introduce the time reversal polarization for noninteracting electrons and show that changes in it define a topological invariant. Our discussion will parallel the theory of charge polarization in insulators.[25–29] In order to establish this connection and to define our notation, we will therefore begin by reviewing that theory, which relates the charge polarization to the average center of Wannier orbitals, which in turn are related to Berry's phase of the Bloch wave functions. We next consider the role of Kramers' degeneracy in time reversal invariant systems and define a corresponding time reversal polarization in terms of the difference between the Wannier centers of Kramers degenerate bands. Finally, we show that the *change* in the time reversal polarization between $t=0$ and $T/2$ of the pumping cycle defines a Z_2 topological invariant that distinguishes a nontrivial Z_2 pump from a trivial cycle.

A. Review of theory of charge polarization

Consider a one-dimensional system with lattice constant $a=1$, length $L=N_c$ with periodic boundary conditions and $2N$ occupied bands. The normalized eigenstates for the nth band can then be written in terms of cell periodic Bloch functions as

$$|\psi_{n,k}\rangle = \frac{1}{\sqrt{N_c}} e^{ikx} |u_{n,k}\rangle. \tag{3.1}$$

We may define Wannier functions associated with each unit cell associated with lattice vector R as

$$|R,n\rangle = \frac{1}{2\pi} \int dk\, e^{-ik(R-r)} |u_{k,n}\rangle. \tag{3.2}$$

The Wannier functions are not unique because they depend on a gauge choice for $|u_{k,n}\rangle$. In addition to changing the phases of the individual wave functions, the wave functions can be mixed by a general U$(2N)$ transformation of the form

$$|u_{k,n}\rangle \to \sum_m U_{nm}(k) |u_{k,m}\rangle. \tag{3.3}$$

After this transformation, $|u_{k,n}\rangle$ need no longer be the individual eigenstates of the Hamiltonian, but rather should be interpreted as basis vectors spanning the space spanned by the $2N$ occupied eigenstates. The Slater determinant of the $2N$ wave functions is unchanged up to a phase.

Marzari and Vanderbilt[29] have provided a prescription for choosing $U_{nm}(k)$ to optimally localize the Wannier wave functions. Here, however, we are concerned with the total charge polarization, which is insensitive to the details of $U_{nm}(k)$. The polarization is given by the sum over all of the bands of the center of charge of the Wannier states associated with $R=0$, and may be written[25,26]

$$P_\rho = \sum_n \langle 0,n|r|0,n\rangle = \frac{1}{2\pi}\oint dk\mathcal{A}(k), \qquad (3.4)$$

where the U(1) Berry's connection is given by

$$\mathcal{A}(k) = i\sum_n \langle u_{k,n}|\nabla_k|u_{k,n}\rangle. \qquad (3.5)$$

The integral is over the Brillouin zone from $k=-\pi$ to π. If we require that the wave function $|\psi_{n,k}\rangle$ be defined continuously in the reduced zone scheme, so that $|\psi_{n,-\pi}\rangle = |\psi_{n,\pi}\rangle$, then $\mathcal{A}(-\pi)=\mathcal{A}(\pi)$, and the integral may be considered to be on a *closed* loop, despite the fact that $|u_{n,k}\rangle$ is discontinuous from $-\pi$ to π.[26] Under a U($2N$) transformation that preserves this continuity P_ρ is invariant up to a lattice constant. For a transformation in which the U(1) phase of $U_{mn}(k)$ advances by $2\pi m$ when k advances around the Brillouin zone, $P_\rho \to P_\rho + m$. This reflects the fact that the polarization can only be defined up to a lattice vector.

Changes in the polarization induced by a continuous change in the Hamiltonian $H[t]$ are, however, well defined. Thus, if the wave functions $|u_{k,n}(t)\rangle$ are defined *continuously* between t_1 and t_2 for all k in the Brillouin zone, then we may write

$$P_\rho[t_2] - P_\rho[t_1] = \frac{1}{2\pi}\left[\oint_{c_2} dk\mathcal{A}(t,k) - \oint_{c_1} dk\mathcal{A}(t,k)\right], \qquad (3.6)$$

where $c_{1(2)}$ is the loop $k=-\pi$ to π for fixed $t=t_{1(2)}$. Using Stokes theorem, this can be written as an integral of the Berry curvature,

$$\mathcal{F}(t,k) = i\sum_n [\langle \nabla_t u_{k,n}(t)|\nabla_k u_{k,n}(t)\rangle - \text{c.c.}] \qquad (3.7)$$

over the surface τ_{12} of the cylinder spanned by k and t bounded by c_1 and c_2,

$$P_\rho[t_2] - P_\rho[t_1] = \frac{1}{2\pi}\int_{\tau_{12}} dt\, dk\mathcal{F}(t,k). \qquad (3.8)$$

For a periodic cycle $H[t+T]=H[t]$, the change in the polarization over one cycle, $P_\rho(T)-P_\rho(0)$, is given by the integral in Eq. (3.8) over the entire torus defined by t and k. This quantity is an integer and defines the first Chern number associated with the wave function $|u_{k,n}(t)\rangle$ on the torus. The Chern number characterizes the charge pumped in each cycle. For a cycle that satisfies the time reversal constraint in Eq. (1.2), $\mathcal{F}(-t,-k)=-\mathcal{F}(t,k)$, so the Chern number is equal to zero.

B. Time reversal polarization for Kramers degenerate bands

Consider now a time reversal invariant system. The time reversal operator has the form

$$\Theta = e^{i\pi S_y/\hbar}K, \qquad (3.9)$$

where S_y is the spin operator and K is complex conjugation. Since $\Theta^2=-1$ for spin-$\frac{1}{2}$ electrons, it follows from Kramers' theorem that every Bloch state at wave vector k is degenerate with a time reversed Bloch state. Therefore, the energy bands come in pairs, which are degenerate at the two time reversal invariant points $k^*=0$ and π, as shown in Fig. 2. Note that in the presence of spin-orbit interactions, these bands *cannot* be labeled with spin quantum numbers.

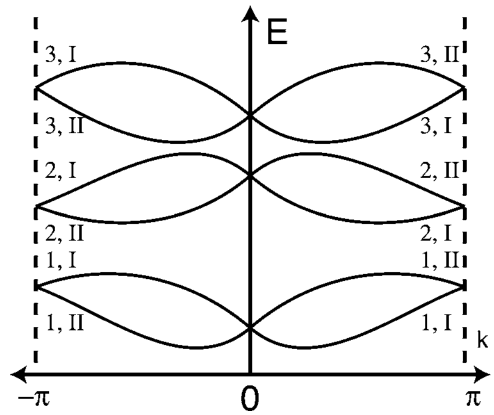

FIG. 2. Schematic one-dimensional band structure with spin-orbit interactions. The energy bands come in time reversed pairs which are degenerate at $k=0$ and π.

In Sec. III A, we related the charge polarization as the sum of the Wannier centers of all of the bands. Kramer's theorem guarantees, however, that the Wannier states come in Kramer's degenerate pairs, in which each pair has the same center. The idea is therefore to keep track of the center of *one* of the degenerate Wannier states per pair by defining a "partial polarization." This will contain more information than Eq. (3.4), which is the sum over both states.

For simplicity we assume that there are no degeneracies other than those required by time reversal symmetry. Therefore, the $2N$ eigenstates may be divided into N pairs that satisfy

$$|u^{\mathrm{I}}_{-k,\alpha}\rangle = -e^{i\chi_{k,\alpha}}\Theta|u^{\mathrm{II}}_{k,\alpha}\rangle$$

$$|u^{\mathrm{II}}_{-k,\alpha}\rangle = e^{i\chi_{-k,\alpha}}\Theta|u^{\mathrm{I}}_{k,\alpha}\rangle, \qquad (3.10)$$

where $\alpha=1,\ldots,N$. The second equation follows from the first, along with the property $\Theta^2=-1$. As shown in Fig. 2, these bands are defined continuously at the degeneracy points $k^*=0,\pi$. This representation is not invariant under the general U($2N$) transformation (3.3). However, that invariance will be restored below.

We define Wannier states associated with these two sets of bands along with the corresponding Wannier centers. By analogy with Eq. (3.4), the partial polarization associated with one of the categories $s=$I or II may then be written

$$P^s = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\mathcal{A}^s(k), \qquad (3.11)$$

where

$$\mathcal{A}^s(k) = i\sum_\alpha \langle u^s_{k,\alpha}|\nabla_k|u^s_{k,\alpha}\rangle. \tag{3.12}$$

The partial polarizations are clearly invariant (up to a lattice translation) under changes in the phases of $|u^{\mathrm{I}}_{k,\alpha}\rangle$ and $|u^{\mathrm{II}}_{k,\alpha}\rangle$. However, they appear to depend on the arbitrary choice of the labels I and II assigned to each band. We now show that the partial polarizations (3.11) can be written in a form that is invariant under a general U($2N$) transformation of the form (3.3). To make this invariance explicit for P_{I}, we treat the portions of the integral for positive and negative k separately,

$$P^{\mathrm{I}} = \frac{1}{2\pi}\int_0^\pi dk[\mathcal{A}^{\mathrm{I}}(k) + \mathcal{A}^{\mathrm{I}}(-k)]. \tag{3.13}$$

For the second term, we use the time reversal constraint (3.10) along with the fact that $\langle \Theta u^{\mathrm{II}}_{k,\alpha}|\nabla_k|\Theta u^{\mathrm{II}}_{k,\alpha}\rangle = -\langle u^{\mathrm{II}}_{k,\alpha}|\nabla_k|u^{\mathrm{II}}_{k,\alpha}\rangle$ to write

$$\mathcal{A}^{\mathrm{I}}(-k) = \mathcal{A}^{\mathrm{II}}(k) - \sum_\alpha \nabla_k\chi_{k,\alpha}. \tag{3.14}$$

It then follows that

$$P^{\mathrm{I}} = \frac{1}{2\pi}\left[\int_0^\pi dk\mathcal{A}(k) - \sum_\alpha(\chi_{\pi,\alpha} - \chi_{0,\alpha})\right]. \tag{3.15}$$

The first term is expressed in terms of Berry's connection $\mathcal{A}=\mathcal{A}^{\mathrm{I}}+\mathcal{A}^{\mathrm{II}}$. However, since the path of integration is not closed, the second term is necessary to preserve gauge invariance. The second term can be rewritten in a suggestive manner by introducing the U($2N$) matrix, which relates the time reversed wave functions,

$$w_{mn}(k) = \langle u_{-k,m}|\Theta|u_{k,n}\rangle. \tag{3.16}$$

In the representation (3.10), w_{mn} is a direct product of 2×2 matrices with $e^{i\chi_{k,\alpha}}$ and $-e^{i\chi_{-k,\alpha}}$ on the off-diagonal. At $k=0$ and π, w_{mn} is *antisymmetric*. An antisymmetric matrix may be characterized by its Pfaffian, whose square is equal to the determinant. We then find that

$$\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]} = \exp\left(i\sum_\alpha(\chi_{\pi,\alpha} - \chi_{0,\alpha})\right). \tag{3.17}$$

Thus, the second term in Eq. (3.15) can be expressed in terms of Pf[w]. This leads to

$$P^{\mathrm{I}} = \frac{1}{2\pi}\left[\int_0^\pi dk\,\mathcal{A}(k) + i\log\left(\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right)\right]. \tag{3.18}$$

Using the identity $\mathrm{Pf}[XAX^T]=\det[X]\mathrm{Pf}[A]$, it can be shown that under the U($2N$) transformation (3.3), $\mathrm{Pf}[w] \to \mathrm{Pf}[w]\det[U]$. Both terms in Eq. (3.18) are thus clearly SU($2N$) invariant. Moreover, under a U(1) transformation, the two terms compensate one another, so P^{I} is U($2N$) invariant. Like the charge polarization (3.4), P^{I} is only defined modulo a lattice vector. This is reflected in the ambiguity of the imaginary part of the log in Eq. (3.18) as well as the dependence of gauge transformations where the phase of $|u_{k,n}\rangle$ advances by 2π for $0<k<\pi$.

A similar calculation can be performed for P^{II}, and it is clear from time reversal symmetry that $P^{\mathrm{II}}=P^{\mathrm{I}}$ modulo an integer, reflecting Kramers' pairing of the Wannier states. From Eqs. (3.4) and (3.11), the charge polarization is given by the sum of the two partial polarizations,

$$P_\rho = P^{\mathrm{I}} + P^{\mathrm{II}}. \tag{3.19}$$

We now define the *time-reversal polarization* as the difference

$$P_\theta = P^{\mathrm{I}} - P^{\mathrm{II}} = 2P^{\mathrm{I}} - P_\rho. \tag{3.20}$$

This then has the form

$$P_\theta = \frac{1}{2\pi}\left[\int_0^\pi dk\,\mathcal{A} - \int_{-\pi}^0 dk\,\mathcal{A} + 2i\log\left(\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right)\right]. \tag{3.21}$$

This may be written more compactly in terms of w_{mn} as

$$P_\theta = \frac{1}{2\pi i}\left[\int_0^\pi dk\,\mathrm{Tr}[w^\dagger\nabla_k w] - 2\log\left(\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right)\right]. \tag{3.22}$$

This can be simplified further by noting that the first term gives the winding of the U(1) phase of w_{mn} between 0 and π. Thus,

$$P_\theta = \frac{1}{2\pi i}\left[\int_0^\pi dk\,\nabla_k\log\det[w(k)] - 2\log\left(\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right)\right]. \tag{3.23}$$

Since $\det[w]=\mathrm{Pf}[w]^2$, this quantity is an integer, and due to the ambiguity of the log, this integer is only defined modulo 2. Even and odd integers are distinct, however, and determine whether $\mathrm{Pf}[w(k)]$ is on the same branch or opposite branch of $\sqrt{\det[w(k)]}$ at $k=0$ and π. An alternative way of writing it is thus,

$$(-1)^{P_\theta} = \frac{\sqrt{\det[w(0)]}}{\mathrm{Pf}[w(0)]}\frac{\sqrt{\det[w(\pi)]}}{\mathrm{Pf}[w(\pi)]}, \tag{3.24}$$

where the branches of $\pm\sqrt{\det[w]}$ are chosen such that the branch chosen at $k=0$ evolves continuously along the path of integration in Eq. (3.23) into the branch chosen at $k=\pi$, eliminating the ambiguity of the square root.

Equations (3.21)–(3.24) are among the principal results of this paper, and can be regarded as a generalization accounting for time reversal symmetry of Berry's phase formulation of the charge polarization.[26] The Z_2 time reversal polarization P_θ defines two distinct polarization states. In the next section, we will argue that the value of P_θ is related to the presence or the absence of a Kramers degenerate state at the end of a finite system. As is the case for P_ρ, the value of P_θ is not meaningful by itself, because a gauge transformation $|u^{\mathrm{I}}_k\rangle \to e^{ik}|u^{\mathrm{I}}_k\rangle$ changes its value. Equivalently, the presence or absence of a Kramers degeneracy at the end cannot be determined from the state in the bulk, since it will depend on how the crystal is terminated. Nonetheless, the two values of P_θ are topologically distinct in the sense that the value of P_θ

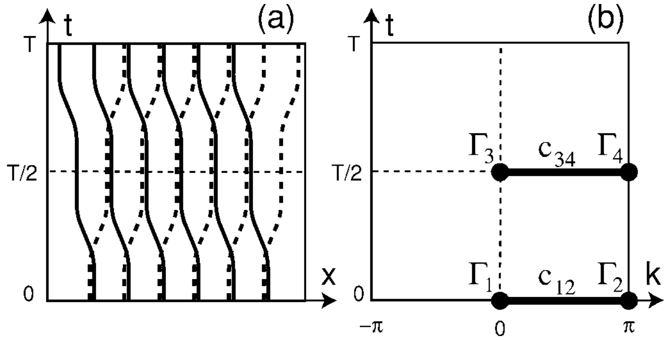

FIG. 3. (a) Schematic diagram showing the evolution of the centers of the time reversed pairs of Wannier states as a function of t. Between $t=0$ and $T/2$, the Wannier states "switch partners," resulting in the appearance of unpaired Wannier states at the end. (b) The torus defined by k and t, with the four time reversal invariant points Γ_i connected by paths c_{12} and c_{34}.

cannot be altered by a continuous change in the Hamiltonian that preserves time reversal symmetry. However, in the next section we will argue that an adiabatic change in the Hamiltonian that preserves time reversal symmetry at the end points—but not in between—leads to a well defined change in P_θ. This change defines a topological classification of distinct pumping procedures.

C. Z_2 invariant

In the previous subsection, we focused on a time reversal invariant Hamiltonian, which occurs at $t=0$ and $T/2$ in our pumping cycle. We now consider the continuous evolution of the Hamiltonian through the cycle and show that the change in the time reversal polarization which occurs in *half* the cycle defines a Z_2 topological invariant, which distinguishes a Z_2 spin pump from a trivial cycle.

This physical meaning of this invariant is easiest to see pictorially by considering the shift in the Wannier centers in the course of one cycle. Figure 3(a) depicts the centers of the occupied Wannier orbitals as a function of t. At $t=0$, $T/2$, and T, time reversal symmetry requires that the Wannier states come in time reversed pairs. However, in going from $t=0$ to $T/2$, the Wannier states "switch partners." In this process, the time reversal polarization, which tracks the difference between the positions of the time reversed Wannier states, changes by one. In addition, this switching results in the appearance of an unpaired occupied Wannier state at each end. Since the Wannier states come in pairs, there must be twofold Kramers degeneracy associated with each end, resulting in a total degeneracy of four.

When the system evolves from $t=T/2$ to T, there is another switch, and the time reversal polarization returns to its original value. However, since $H[t]=\Theta H[T-t]\Theta^{-1}$, the system with open ends does not return to its original state at $t=0$ but its ends are in an excited state because of the level crossing at $t=T/2$.

We now relate the occurrence of this nontrivial pumping cycle to a topological property of the *bulk ground state* as a function of t. We thus consider the change in the time reversal polarization, $P_\theta(t)$, between $t=0$ and $T/2$. Note that though P_θ is not gauge invariant, the *change* in P_θ is gauge invariant. This difference

$$\Delta = P_\theta(T/2) - P_\theta(0) \bmod 2 \tag{3.25}$$

defines a Z_2 topological invariant that characterizes the mapping from the torus defined by k and t to the wave functions: $|u_{k,n}(t)\rangle$. From Eq. (3.24), we may write this invariant as

$$(-1)^\Delta = \prod_{i=1}^{4} \frac{\sqrt{\det[w(\Gamma_i)]}}{\mathrm{Pf}[w(\Gamma_i)]}. \tag{3.26}$$

Here Γ_i are the four "time reversal invariant points" on the torus shown in Fig. 3(b). The branches of the square root are chosen as in Eq. (3.24) by continuously evolving $\sqrt{\det[w(k,t)]}$ along the paths c_{12} and c_{34}. In order to apply this formula, it is crucial for the wave functions to be defined *continuously* on the torus. It is always possible to find such smoothly defined wave functions via a transformation of the form (3.3) because the Chern number, which is the obstruction to doing so, is equal to zero.

In the Appendix, we will relate different mathematical formulations of this invariant. We will first show that it can be interpreted as an obstruction to defining continuous wave functions provided an additional constraint relating the wave functions at time reversed points is enforced. This leads to a different formula for the invariant, which can be expressed in terms of Berry's curvature $\mathcal{F}$ and Berry's connection $\mathcal{A}$. We will then prove that Eq. (3.26) is equivalent to the formula for the invariant introduced in Ref. 13.

IV. ELECTRON INTERACTIONS AND BOSONIZATION

The preceding discussion has focused on noninteracting electrons. An important question is therefore whether these ideas apply to interacting systems. The presence or absence of a ground-state Kramers degeneracy associated with the ends of a finite interacting time reversal invariant system is clearly a well-posed yes or no question. This suggests that the time reversal polarization is a well defined quantity, at least for nonfractionalized phases for which the ground state with periodic boundary conditions is nondegenerate. Therefore, we believe the topological distinction of the Z_2 pump is still present with interactions.

Calculating the time reversal polarization for interacting electrons is more subtle than for noninteracting electrons. One possible approach would involve characterizing the *entanglement entropy*, as in Ref. 31, which is sensitive to the presence or absence of end states. In this section, we adopt a simpler approach by studying an interacting version of the model introduced in Sec. II using Abelian bosonization. We find that bosonization provides a natural description of the time reversal polarization.

We begin with a continuum version of Eq. (2.1) described by the Hamiltonian density,

$$H = \psi^\dagger(iv_F\tau^z\partial_x + h_{\rm st}\tau^x\sigma^z + \Delta t_{\rm st}\tau^y + i\vec{e}_{\rm so}\cdot\vec{\sigma}\tau^z)\psi. \tag{4.1}$$

Here $\psi_{a\alpha}$ is a four-component field, where the left and right moving fields $a=L,R$ are specified by the eigenvalues of τ^z_{ab}

and the spin $\alpha=\uparrow\downarrow$ by $\sigma^z_{\alpha\beta}$. We now bosonize according to

$$\psi_{a\alpha} = \frac{1}{\sqrt{2\pi x_c}} e^{i\phi_{a\alpha}}, \tag{4.2}$$

where x_c is a short-distance cutoff. Define charge/spin variables so that $\phi_{\uparrow/\downarrow\alpha}=\phi_{\rho\alpha}\pm\phi_{\sigma\alpha}$, and charge/current variables (with $\mu=\rho,\sigma$) as $\phi_{\mu L/R}=\varphi_\mu\pm\theta_\mu$. These obey $[\partial_x\theta_\mu(x),\varphi_{\mu'}(x')]=i(\pi/2)\delta_{\mu\mu'}\delta(x-x')$.

The bosonized Hamiltonian then has the form (2.1) with

$$H_0 = \frac{v_F}{4\pi}[(\partial_x\varphi_\rho)^2 + (\partial_x\theta_\rho)^2 + (\partial_x\varphi_\sigma)^2 + (\partial_x\theta_\sigma)^2], \tag{4.3}$$

$$V_h = \frac{h_{\rm st}}{2\pi x_c}\sin 2\theta_\rho \sin 2\theta_\sigma, \tag{4.4}$$

$$V_t = \frac{\Delta t_{\rm st}}{2\pi x_c}\sin 2\theta_\rho \cos 2\theta_\sigma, \tag{4.5}$$

and

$$V_{\rm so} = \frac{e^z_{\rm so}}{\pi}\partial_x\varphi_\sigma + \frac{e^x_{\rm so}}{2\pi x_c}\sin 2\theta_\sigma \cos 2\varphi_\sigma + \frac{e^y_{\rm so}}{2\pi x_c}\sin 2\theta_\sigma \sin 2\varphi_\sigma. \tag{4.6}$$

In the absence of the spin-orbit term, the spin sector of this Hamiltonian (when θ_ρ is pinned at $\pi/4$) is equivalent to Shindou's model.[4] This Hamiltonian describes an insulating phase in which both θ_ρ and θ_σ are pinned.

First focus on the case $h_{\rm st}=0$, where the Hamiltonian is time reversal invariant. If we choose a gauge such that $\Theta\psi\Theta^{-1}=\tau^x\sigma^y\psi^*$, the behavior of these operators under time reversal can be deduced,

$$\Theta\theta_\rho\Theta^{-1} = \theta_\rho, \quad \Theta\varphi_\rho\Theta^{-1} = -\varphi_\rho,$$

$$\Theta\theta_\sigma\Theta^{-1} = -\theta_\sigma, \quad \Theta\varphi_\sigma\Theta^{-1} = \varphi_\sigma + \pi/2. \tag{4.7}$$

The time reversal invariance of the Hamiltonian when $h_{\rm st}=0$ can easily be verified. It is now straightforward to consider time reversal invariant interaction terms, such as $(\partial_x\theta_\rho)^2$, $(\partial_x\theta_\sigma)^2$, $\cos 4\theta_\rho$, $\cos 4\theta_\sigma$, $\cos 4\varphi_\sigma$, etc. Provided these interaction terms (as well as $V_{\rm so}$ defined above) are not too large, the system will retain its bulk gap and be in a phase in which θ_ρ and θ_σ are pinned.

We now identify the time reversal polarization with

$$P_\theta = 2\theta_\sigma/\pi \bmod 2. \tag{4.8}$$

The apparent dependence of P_θ on the spin quantization axis is an Artifact of Abelian bosonization. In fact, P_θ is SU(2) invariant. This can be seen by noting that global spin rotations are generated by $S^z\sim\int dx\,\partial_x\theta_\sigma$ and $S^\pm\sim\int dx\exp\pm 2i\phi_\sigma$. The latter obeys $[\theta_\sigma,S^\pm]=\pm\pi S^\pm$, so that $[P_\theta,S^\pm]=0$. It can further be seen that even in the presence of spin nonconserving terms in $V_{\rm so}$ as well as the interaction terms discussed above, $[P_\theta,H]=0$. Since $\Theta P_\theta\Theta^{-1}=-P_\theta \bmod 2$, there are two distinct possible values for the time reversal polarization: $\langle P_\theta\rangle=0$ or 1. Thus P_θ can be used to classify time reversal invariant insulating states.

Consider a finite system with ends. We now argue that the value of P_σ determines the presence or absence of Kramers degenerate states at the ends. The end of a one-dimensional system at $x=0$ must be characterized by a boundary condition for $\theta_\sigma(x=0)$. Time reversal symmetry limits the possible values to $\theta_\sigma(x=0)=n\pi$. The value of n, however, depends on how the lattice is terminated. First suppose that $n=0$. Then, when $P_\sigma=1$, the pinning of θ_σ in the bulk is not consistent with the boundary condition. The closest it can be is $\langle\theta_\sigma\rangle=\pm\pi$. Thus, near the end there must be a kink of $\pm\pi$ in θ_σ at the end. Time reversal symmetry requires these two possibilities to be degenerate, so there is a Kramers degeneracy of two at the end. On the other hand, when $P_\sigma=0$, the bulk energy gap is "consistent" with the boundary condition, allowing for $\theta_\sigma(x)=0$ everywhere. The ground state in this case is unique.

We thus conclude that bosonization provides an alternative approach for formulating the time reversal polarization in terms of θ_σ, just as it allows for a formulation of the charge polarization $P_\rho=\theta_\rho/\pi$. This suggests that the topological distinction of the Z_2 spin pump remains in the presence of electron interactions.

V. DISCUSSION

A. Relation to the quantum spin Hall effect

The quantum spin Hall phase introduced in Ref. 12 is a phase of a two-dimensional electron system. In a manner analogous to Laughlin's construction for the quantum Hall effect,[32] this phase, when compactified onto a cylinder, defines a Z_2 pump of the sort studied in this paper. In this section, we outline the implications of the present work for the quantum spin Hall effect. We begin by relating the Z_2 index introduced in Sec. III to the index that distinguishes the quantum spin Hall phase from a band insulator. We then discuss the presence or absence of gapless edge states in the quantum spin Hall effect. Finally, we comment on an alternative topological characterization of the quantum spin Hall effect in terms of a "Chern number matrix" that has recently been proposed by Sheng *et al.*[30]

1. Z_2 classification of the quantum spin Hall phase

For noninteracting electrons, the electronic phase of a two-dimensional system with a bulk gap is characterized by the wave functions defined on the Brillouin zone torus, $|u_n(k_x,k_y)\rangle$. The relationship between the one-dimensional Z_2 pump and the two-dimensional quantum spin Hall effect can be established by the identification of (k,t) with (k_x,k_y). Equation (1.2) then reflects the time reversal invariance of the two-dimensional Hamiltonian. As we prove in the Appendix, the Z_2 topological index introduced in Ref. 13 is equivalent to the Z_2 index characterizing the pump. The considerations of this paper provide a natural physical interpretation of this index in terms of the change in the time reversal polarization in half of the cycle.

In addition, our observation that the time reversal polarization is related to the presence or absence of a Kramers

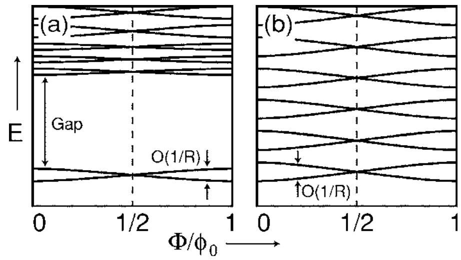

FIG. 4. Schematic plots of the many-particle eigenstates of a cylindrical quantum spin Hall system of radius R as a function of the magnetic flux threading the cylinder. In each case, there is a Kramers degeneracy when the flux Φ is equal to $h/2e$. (a) There exist gapless edge excitations, whose energy level spacing goes to zero for $R \to \infty$. (b) There is an edge excitation gap that remains finite for $R \to \infty$, but the ground state is doubly degenerate.

degeneracy at the end suggests that the Z_2 classification of time reversal invariant two-dimensional ground states transcends the noninteracting model for which it was derived. This means that the quantum spin Hall effect describes a phase that is distinct from a band insulator even in the presence of electron-electron interactions.

2. Edge states or not?

In the regular quantum Hall effect, the topological structure of the bulk state guarantees the existence of gapless edge excitations. The nontrivial Z_2 invariant, however, does *not* guarantee gapless edge states. As shown by Wu *et al.*[17] and Xu *et al.*,[18] when the interactions at the edge are sufficiently strong, the edge can undergo a transition that opens a gap. The considerations of this paper allow us to prove that *either* there are gapless edge excitations *or* there is a ground-state degeneracy at the edge associated with the breaking of time reversal symmetry.

To establish this proposition, consider the many-particle eigenstates of the quantum spin Hall phase on a cylinder as a function of the magnetic flux through the cylinder. When the radius R of the cylinder is large, then the $O(1/R)$ change in the energy of the many-particle eigenstates when one-half of a flux is inserted will be much less than any energy gap. But in the quantum spin Hall state, the nontrivial Z_2 index requires the ground state to have a Kramers degeneracy at either $\Phi=0$ or $\Phi=\phi_0/2$, but not both. Thus there are two possibilities as schematically illustrated in Fig. 4. Either there are edge states with energy $O(1/R)$ that become gapless for $R\to\infty$, or the ground state is degenerate for $R\to\infty$ and split by at most $O(1/R)$ by the magnetic flux.

This required ground-state degeneracy distinguishes the quantum spin Hall phase from that of a band insulator. Unlike a band insulator, the quantum spin Hall state in a system with edges *cannot* have a unique ground state with a gap for all excitations.

3. Other proposed classifications of the quantum spin Hall effect

We now comment on a different topological classification of the quantum spin Hall effect proposed by Sheng *et al.*[30] These authors defined a matrix of Chern numbers by considering a system with a generalized class of periodic boundary conditions. Specifically, they considered boundary conditions of the form $\Phi(\ldots,\mathbf{r}_{i\alpha}+\mathbf{L}_{\mathbf{j}},\ldots)=\exp(i\theta_j^{\alpha})\Phi(\ldots,\mathbf{r}_{i\alpha},\ldots)$, where $\mathbf{L}_{j=x,y}$ define the periodicity and $\theta_j^{\alpha=\uparrow,\downarrow}$ are *independent* phase twists for the up and down spins. They then characterized the topological classes of the ground-state wave function as a function of these phase twists, and defined a matrix of Chern numbers, $C^{\alpha,\beta}$.

Sheng *et al.* argued that this classification contains more information than the Z_2 classification because it distinguishes quantum spin Hall states which belong to the same Z_2 class. This can be illustrated by looking at the continuum version of the graphene model introduced in Ref. 12, described by the Hamiltonian

$$H = \psi^\dagger[-iv_F(\sigma_x\tau_z\partial_x + \sigma_y\partial_y) + \Delta_{so}\sigma_z\tau_z s_z]\psi. \qquad (5.1)$$

Here, in the notation of Ref. 12, σ_z describes the sublattice of the honeycomb lattice, τ_z describes the two inequivalent valleys at the corners of the Brillouin zone, and s_z describes the spin. When Δ_{so} is nonzero, the system is in a quantum spin Hall phase and belongs to the nontrivial Z_2 class. Sheng *et al.*[30] argued that the *sign* of Δ_{so} defines two distinct phases that are distinguished by the matrix of Chern numbers.

When s_z is conserved this is certainly correct, and the Chern number matrix can be viewed as independent Chern numbers for the up and down spins. However, when spatial symmetries are relaxed and spin is not conserved, this distinction is no longer meaningful. The two phases discussed above are in fact the *same* phase because they can be continuously transformed into one another without closing the gap. Specifically, consider the more general spin-orbit interaction that preserves the energy gap,

$$\sigma_z\tau_z s_z \to \sigma_z\tau_z(\vec{s}\cdot\hat{n}). \qquad (5.2)$$

When the unit vector $\hat{n}$ is continuously varied from $+\hat{z}$ to $-\hat{z}$, the two "phases" are connected. Of course, the process of connecting these phases requires the breaking of the C_3 lattice symmetry of graphene. But in general, disorder will break all spatial symmetries, so one cannot rely on a spatial symmetry to protect a topological property.

This presents a conundrum because the Chern matrix formulation distinguishes the two states with distinct topological integers, even when the C_3 symmetry is explicitly violated. What happens to these integers when the continuous path in Eq. (5.2) is adiabatically followed? The answer is that somewhere along the path the energy gap must vanish at the *edge* where the twisted spin boundary condition is imposed.[33]

The spin phase twist imposed by Sheng *et al.* can be decomposed into a U(1) part $\theta_\rho=\theta_\uparrow+\theta_\downarrow$ and a "spin" part $\theta_\sigma=\theta_\uparrow-\theta_\downarrow$. The spin phase twist θ_σ is fundamentally different from θ_ρ when the bulk Hamiltonian does not commute with the S_z. The boundary where the spin phase twist is imposed is physically different from the rest of the system, and the spectrum of the Hamiltonian will in general be different for different values of θ_σ. In contrast, the location of the charge phase twist θ_ρ introduced by Niu and Thouless[24] can be moved around by performing a local gauge transformation without changing the spectrum. Since the vector poten-

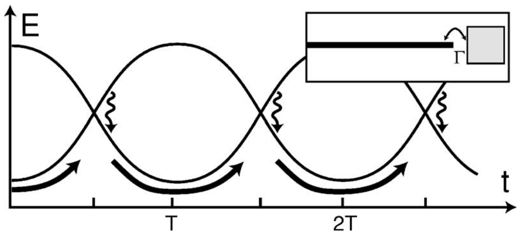

FIG. 5. Evolution of one end of a Z_2 pump that is weakly connected to a lead as shown in the inset. For $t \gtrsim T/2$, the excited state of the pump can relax by creating an odd under time reversal excitation in the lead, which generically will change the spin of the reservoir.

tial can be spread out over the circumference $2\pi R$ of the torus, the change in the spectrum due changing θ_ρ can be at most $O(1/R)$. In contrast, if the spin phase twist is spread out over the circumference, changing θ_σ changes the Hamiltonian by an amount of order 1. The spectrum need not be close to that of the physical Hamiltonian.

We conclude that the additional topological structure implied by the Chern number matrix is a property of the *boundary* where the twisted phase condition is imposed rather than a property of the bulk two-dimensional phase. The bulk quantum spin Hall effect is classified by the Z_2 invariant alone.

B. Can the Z_2 spin pump pump spin?

Is the Z_2 pump we introduced a spin pump? Since an isolated Z_2 pump returns to its original state after two cycles, the simple answer to this question is no. However, any functioning pump must be connected to reservoirs into which the pump can pump. In this section, we briefly consider the effect of connecting the Z_2 spin pump to reservoirs. We conclude that the Z_2 pump *does* pump spin, though the spin pumped per cycle is not quantized. Moreover, we argue that when the coupling to the reservoirs is weak, the Z_2 topological structure of the pump is essential for a nonzero spin to be pumped. For stronger coupling, however, the Z_2 structure is not essential.

We consider a simple case where the reservoirs can be described by noninteracting electrons with vanishing spin-orbit interaction. We first suppose the coupling to the reservoir is weak, so that the level width Γ induced in the pump due the coupling is small compared to the energy gap Δ. However, we require the coupling Γ to be large compared to the pumping rate, as well as any inelastic scattering rate for the end states. In the limit

$$\hbar/T, \hbar/\tau_\varphi \ll \Gamma \ll \Delta, \tag{5.3}$$

the eigenstates of the pump maintain their integrity, though coupling to the reservoirs allows transitions between different states.

As illustrated in Fig. 5, there is a point in every cycle $t = (n+1/2)T$ where the ground state of the pump becomes degenerate. This degeneracy is due to the end states, which are in proximity to the reservoir. For $t \gtrsim (n+1/2)T$, the pump is in an *excited* state. Coupling to the reservoir, however, allows the pump to relax back to its ground state. This relaxation, however, must involve a process in the reservoir that is *odd* under time reversal. Generically, this will involve changing the expectation value of the spin of the reservoir. The spin transferred to the reservoir need not be quantized, because the end states are not necessarily spin eigenstates and the coupling to the reservoirs need not conserve spin. The expectation value of the transferred spin could even be equal to zero, but generically, it will be of order $\hbar$.

In this weak-coupling limit, it is clear that the Z_2 structure of the pumping cycle is essential because it guarantees the level crossing in the end states. If the end states did not cross, then there would be no transitions, and the spin in the reservoirs would be unchanged after a complete cycle. However, finite coupling to the leads relaxes this requirement. Suppose that the time reversal symmetry is weakly broken at $t = T/2$, so that there is a small anticrossing of magnitude δ. In this case, the Z_2 character of the cycle is lost. But if $\delta \ll \Gamma$, then the states have no way of "knowing" about the anticrossing, and the pump proceeds as if $\delta = 0$.

This reflects the fact that spin can be introduced into a reservoir that is connected to an insulating material when the insulator is deformed through a periodic cycle. The spin injected can be expressed in terms of the unitary reflection matrix $\hat{r}(t)$ for electrons at the Fermi energy in the reservoir,[34] which in general depends on the Hamiltonian $H(t)$ of the insulator,

$$\Delta\vec{S} = \frac{1}{2\pi i}\oint dt \mathrm{Tr}\left[\vec{S}\hat{r}^\dagger \frac{d\hat{r}}{dt}\right]. \tag{5.4}$$

In general, this quantity is nonzero. The difficulty is coming up with a cycle in an insulating material for which ΔS is not very small. The Z_2 pump accomplishes this by guaranteeing that there is a resonance in the reflection matrix, which occurs when the Kramers degenerate end state appears. Note that this resonance need not involve charge transfer between the reservoir and the insulator. Indeed, if charge fluctuations are suppressed, then the coupling between the end states and the reservoir will resemble the coupling between an impurity spin and the conduction electrons in the Kondo problem. In this case, the resonance in the reflection matrix is analogous to the *Kondo resonance* in the scattering matrix of an impurity, which occurs precisely at the Fermi energy, and signifies the entanglement between the Kramers degenerate impurity spin and the reservoir electrons.

It should be emphasized that the spin added to the reservoir is not a property of the bulk Hamiltonian of the pump, but rather it depends on how the pump is connected to the reservoir. The spin transferred to the reservoirs at the two ends of the pump need not be related. Thus, one cannot view the spin as being pumped along the length of the pump. However, the presence of the end state resonance, which follows from the change in the time reversal polarization, *is* a property of the bulk insulating state. In this sense, the Z_2 pump is a pump for spin.

ACKNOWLEDGMENTS

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APPENDIX A: EQUIVALENT FORMULATIONS OF THE Z_2 INVARIANT

In this appendix, we relate different mathematical formulations of the Z_2 invariant Δ. Our starting point is Eq. (3.25) along with Eqs. (3.21)–(3.24), which express the invariant in terms of the change in the time reversal polarization between $t=0$ and $T/2$. We will first show that Δ can be interpreted as an obstruction to defining wave functions continuously, provided a time reversal constraint is enforced. This will lead to a formula for Δ in terms of the Berry curvature and Berry connection, which will be shown to be equivalent to Eq. (3.25). We will then show that Eq. (3.25) is equivalent to the Z_2 invariant proposed for the quantum spin Hall effect in Ref. 13.

We will use a notation appropriate for the Z_2 pumping problem and consider Bloch wave functions defined continuously on the torus defined by $-\pi<k<\pi$ and $0<t<T$. For the two-dimensional quantum spin Hall effect, we should identify k_x with k and k_y with $2\pi t/T$.

1. Z_2 invariant as an obstruction

It is well known that a nonzero value of the Chern invariant is an obstruction to smoothly defining the wave function throughout the entire torus.[23,35] Instead, wave functions must be defined on overlapping "patches," which are related to each other by a gauge transformation called a "transition function." The Chern number is then related to the winding number of the phase of the transition function around a noncontractable path. For the problem studied in this paper, the Chern number is zero, so there is no obstruction to finding a transformation of the form (3.3), which makes the wave functions smoothly defined on a single patch. However, we will show in this section that if we enforce the *time reversal constraint*

$$|u_\alpha^{\mathrm{I}}(-k,-t)\rangle = \Theta|u_\alpha^{\mathrm{II}}(k,t)\rangle,$$

$$|u_\alpha^{\mathrm{II}}(-k,-t)\rangle = -\Theta|u_\alpha^{\mathrm{I}}(k,t)\rangle, \qquad \text{(A1)}$$

then a nonzero value of the Z_2 invariant is an obstruction in a manner precisely analogous to the Chern number. This constraint means that the gauges for the wave functions at $\pm(k,t)$ are not independent. At the four time reversal invariant points $(k,t)=\Gamma_i$, the allowed transformations of the form (3.3) are restricted to be *symplectic*, $U_{mn}(\Gamma_i)\in \mathrm{Sp}(N)$. That a nonzero value of the Z_2 invariant Δ is inconsistent with this constraint is easy to see because it implies that $\det[w(k,t)]=1$ for all k and t and $\mathrm{Pf}[w(\Gamma_i)]=1$, so Eq. (3.26) trivially gives $\Delta=0$.

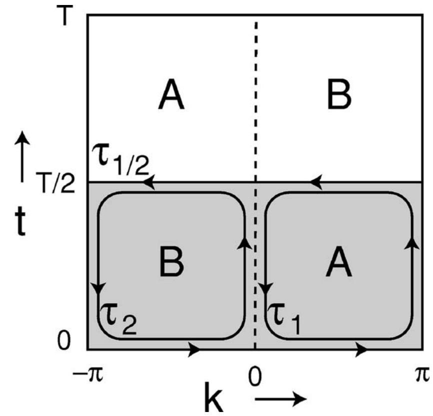

FIG. 6. The torus defined by k and t divided into two patches A and B. The boundaries of the regions τ_1 and τ_2 are shown as well as the boundary of the shaded region, $\tau_{1/2}$.

We will now relate the Z_2 invariant to the winding of the phase of transition functions relating the wave functions on different patches. In addition to establishing the connection between the Z_2 invariant and the Chern invariant, this approach will derive a formula for the Z_2 invariant which expresses it in terms of Berry's connection and curvature. The similarity between the Z_2 invariant and the Chern invariant has been emphasized by Haldane.[36] The formulation of the Z_2 invariant as an obstruction has also been discussed by Roy,[37] though that work did not establish a formula for the invariant.

Suppose that we have wave functions obeying (A1) defined smoothly on two patches in the torus labeled A and B in Fig. 6. In patch A, the wave functions $|u_\alpha^s(k,t)\rangle_A$ are smoothly defined everywhere in the upper left and lower right quadrants of Fig. 6, while for patch B, $|u_\alpha^s(k,t)\rangle_B$ are defined in the upper right and lower left quadrants. In the overlapping regions these different wave functions are related by a U($2N$) transition matrix

$$|u_m(k,t)\rangle_A = t_{mn}^{AB}|u_n(k,t)\rangle_B, \qquad \text{(A2)}$$

where m and n are shorthand for s and α. Consider the change in the U(1) phase of t^{AB} around the closed loop $\partial\tau_1$ in Fig. 6,

$$D=\frac{1}{2\pi i}\oint_{\partial\tau_1} d\ell\, \mathrm{Tr}[t^{AB\dagger}\nabla t^{AB}]. \qquad \text{(A3)}$$

This will clearly be an integer because it is equal to the winding number of the phase of $\det[t^{AB}]$ around the loop $\partial\tau_1$. If D is nonzero and cannot be eliminated by a gauge transformation, then there is an obstruction to smoothly defining the wave functions on a single patch. In what follows, we show that D mod 2 is precisely equal to the Z_2 invariant defined in this paper.

From Eq. (A3), we may write

$$D=\frac{1}{2\pi}\oint_{\partial\tau_1} d\ell(\mathcal{A}^B-\mathcal{A}^A), \qquad \text{(A4)}$$

where $\mathcal{A}^A=\Sigma_{nA} i\langle u_n|\nabla|u_n\rangle_A$ and likewise for $\mathcal{A}^B$. Since $|u_n\rangle_A$ is smoothly defined in the interior of τ_1, we may write it in terms of Berry's flux,

$$\oint_{\partial\tau_1} d\ell\, \mathcal{A}^A = \int_{\tau_1} d\tau\, \mathcal{F}^A. \tag{A5}$$

This cannot be done for $|u_n\rangle_B$, which is not necessarily defined continuously inside τ_1. However, it can be related to Berry's flux through τ_2,

$$\oint_{\partial\tau_1} d\ell\, \mathcal{A}^B = -\oint_{\partial\tau_2} d\ell\, \mathcal{A}^B + \oint_{\partial\tau_{1/2}} d\ell\, \mathcal{A}^B \tag{A6}$$

$$= -\int_{\tau_2} d\tau\, \mathcal{F}^B + \oint_{\partial\tau_{1/2}} d\ell\, \mathcal{A}^B. \tag{A7}$$

Combining these, we thus find the winding number for the transition function can be expressed as an integral involving the Berry connection and the Berry curvature,

$$D = \frac{1}{2\pi}\left[\oint_{\partial\tau_{1/2}} d\ell\, \mathcal{A} - \int_{\tau_{1/2}} d\tau\, \mathcal{F}\right] \bmod 2. \tag{A8}$$

The patch labels can be safely removed because $\mathcal{F}$ is gauge invariant, and the line integral is gauge invariant modulo 2. It is essential that the time reversal constraint (A1) be enforced for this equation to have meaning. If not, then a gauge transformation on patch B can change the line integral by 1, making the formula vacuous. When Eq. (A1) is enforced, an *odd* value of D cannot be gauged away because the phases of $|u^{\mathrm{I}}\rangle$ and $|u^{\mathrm{II}}\rangle$ cannot be independently changed. Thus, $D=1$ mod 2 presents an obstruction to defining wave functions on a single patch.

We now show that this winding number is precisely the same as the invariant Δ. To this end, we rewrite Δ in terms of the *partial polarization* P^{I} defined in Eq. (3.11). Using $P_\theta=2P^{\mathrm{I}}-P_\rho$, we have

$$\Delta = 2[P^{\mathrm{I}}(T/2) - P^{\mathrm{I}}(0)] - [P_\rho(T/2) - P_\rho(0)] \bmod 2. \tag{A9}$$

When Eq. (A1) is enforced, Eq. (3.18) for the partial polarization implies that

$$2[P^{\mathrm{I}}(T/2) - P^{\mathrm{I}}(0)] = \frac{1}{2\pi}\oint_{\partial\tau_{1/2}} d\ell\, \mathcal{A}. \tag{A10}$$

Equation (3.4) shows that

$$P_\rho(T/2) - P_\rho(0) = \frac{1}{2\pi}\int_{\tau_{1/2}} d\tau\, \mathcal{F}. \tag{A11}$$

Combining the two terms thus establishes that $\Delta=D$. The two terms in Eq. (A8) thus acquire physical meaning: The line integral gives twice the change in the partial polarization between $t=0$ and $T/2$, while the surface integral gives the change in the total polarization.

2. Zeros of the Pfaffian

In Ref. 13, the Z_2 invariant was introduced by considering the matrix elements of the time reversal operator,

$$m_{ij}(k,t) = \langle u_i(k,t)|\Theta|u_j(k,t)\rangle. \tag{A12}$$

This should be contrasted with the matrix $w_{ij}(k,t)$ introduced in Sec. III, which can be generalized as a function of t to be

$$w_{ij}(k,t) = \langle u_i(-k,-t)|\Theta|u_j(k,t)\rangle. \tag{A13}$$

At the four time reversal invariant points $(k,t)=\Gamma_{1,2,3,4}=(0,0)$, $(\pi,0)$, $(0,T/2)$, $(\pi,T/2)$, w_{ij} and m_{ij} coincide, but in general they are different. w_{ij} is unitary with $|\det[w]|=1$, while m_{ij} is not unitary. Since $\Theta^2=-1$, m_{ij} is antisymmetric. The Pfaffian of m is therefore defined for all k and t. In Ref. 13, we argued that the Z_2 invariant could be determined by counting the number of zeros of the Pfaffian in half the torus, modulo 2.

To establish the equivalence of this with Eq. (3.25), we begin by rewriting the time reversal polarization P_θ in terms of $\mathrm{Pf}[m(k,t)]$. The key observation to be made is that

$$\det[w(k,t)] = \frac{\mathrm{Pf}[m(k,t)]}{\mathrm{Pf}[m(-k,-t)]^*}, \tag{A14}$$

which can be proved by noting that $m(-k,-t)=w(k,t)m(k,t)^* w(k,t)^T$ and using the identity $\mathrm{Pf}[XAX^T]=\det[X]\mathrm{Pf}[A]$. Introducing $p(k)=\mathrm{Pf}[m(k,t^*)]$ for $t^*=0,T/2$, it follows that $\log\det[w(k,t^*)]=\log p(k)-\log p(-k)^*=i\,\mathrm{Im}[\log p(k)+\log p(-k)]$. Thus we may rewrite Eq. (3.23) as

$$P_\theta = \frac{1}{2\pi i}\left[\int_0^\pi dk \nabla_k[\log p(k) + \log p(-k)] - 2\log\left(\frac{p(\pi)}{p(0)}\right)\right], \tag{A15}$$

where we have used the coincidence of w and m at $k=0$ and π, along with the fact that $|p(0)|=|p(\pi)|=1$. This may be simplified further by changing variables $k\to -k$ in the middle term and writing the last term as an integral from 0 to π. This gives

$$P_\theta = \frac{1}{2\pi i}\int_{-\pi}^{\pi} dk\, \nabla_k \log \mathrm{Pf}[m(k,0)] \bmod 2, \tag{A16}$$

where the integral is now over the closed loop $t=0$, $-\pi<k<\pi$. This expression is only defined modulo 2 because of the ambiguity of the imaginary part of the log in Eq. (A15).

Thus, we have established that P_θ is given by the phase winding of the Pfaffian, $p(k)$ around the 1D Brillouin zone modulo 2. While this quantity is not gauge invariant, the change in it due to continuous evolution between $t^*=0$ and $T/2$ is gauge invariant. This defines the Z_2 topological invariant, which, as in Ref. 13, may be written

$$\Delta = \frac{1}{2\pi i}\oint_{\partial\tau_{1/2}} d\ell\ \nabla\ \log \mathrm{Pf}[m(k,t)] \bmod 2, \tag{A17}$$

where $\partial\tau_{1/2}$ is the boundary of half the torus defined by $-\pi<k<\pi$ and $0<t<T/2$ (see Fig. 6). If $\mathrm{Pf}[m(k,t)]$ has point zeros, then this quantity counts the number of zeros in $\tau_{1/2}$ modulo 2.

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