

# Tuning phase transition between quantum spin Hall and ordinary insulating phases

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An effective theory is constructed for analyzing a generic phase transition between the quantum spin Hall and the insulator phases. Occurrence of degeneracies due to closing of the gap at the transition are carefully elucidated. For systems without inversion symmetry the gap closing occurs at  $\pm\vec{k}_0(\neq\vec{G}/2)$  while for systems with inversion symmetry, the gap can close only at wave numbers  $\vec{k}=\vec{G}/2$ , where  $\vec{G}$  is a reciprocal lattice vector. In both cases, following a unitary transformation which mixes spins, the system is represented by two decoupled effective theories of massive two-component fermions having masses of opposite signs. Existence of gapless helical modes at a domain wall between the two phases directly follows from this formalism. This theory provides an elementary and comprehensive phenomenology of the quantum spin Hall system.

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## I. INTRODUCTION

The intrinsic spin Hall effect (SHE)<sup>1,2</sup> driven by the relativistic spin-orbit interaction and the associated Berry curvature of the Bloch wave functions attracts considerable attention both theoretically and experimentally. In conducting materials such as doped GaAs, the external electric field produces transport current and dissipation, even though the spin current transverse to it is dissipationless. Therefore it is highly desirable to design systems showing the SHE without dissipation. Spin Hall insulator (SHI) has been proposed for this purpose by some of the present authors, and its candidate materials are HgTe, PbTe,  $\alpha$ -Sn, and so forth.<sup>3</sup> These band insulators are predicted to show finite spin Hall conductivity  $\sigma_H^s$ , which is not quantized and depends on parameters in the model Hamiltonian. Later it has been realized that gapless edge modes in semi-infinite systems do not exist in generic cases. These two features, i.e., the nonquantized  $\sigma_H^s$  and the absence of gapless edge modes, are closely related to the absence of conserved spin current in the presence of spin-orbit interaction, i.e., there is no U(1) gauge symmetry for spin current. Therefore it was difficult to distinguish between the SHI and usual insulators.

Recently, Kane and Mele proposed a model for time-reversal ( $T$ ) invariant systems,<sup>4,5</sup> which manifests a finite SHE and demonstrated its distinction from an ordinary insulator due to the topological nature of its ground state. The pertinent  $Z_2$  topology is represented by an integer  $\Delta$  defined for Bloch wavefunctions in the bulk, whose parity distinguishes the relevant phases. Physically,  $\Delta$  is identical with the number of pairs of helical edge modes. In a system with  $\Delta$ =odd, referred to as quantum spin Hall (QSH) system,<sup>4-9,11-15</sup> the odd number of pairs of helical edge modes is robust against weak nonmagnetic disorder and interactions.<sup>16,17</sup> When  $\Delta$ =even, gapless edge modes can hy-

bridize each other and a gap will open even at the edge. The system is then referred to as spin Hall insulator (SHI). Transitions between phases with  $\Delta$ =even (SHI) and  $\Delta$ =odd (QSH) occur only when the gap is closed by tuning parameters of the model. Constructing a theory for analyzing these transitions is a challenge of paramount interest.

In this paper, we develop an effective continuum theory for phase transitions between QSH and SHI systems in 2D and discuss (i) classification of the possible types of transition, (ii) existence of gapless helical edge modes, and (iii) the change of the  $Z_2$  topological number at the transition. The basic idea is that effective continuum theory focusing on the vicinity of the gap-closing points at the transition can be constructed even though characterization of each phase requires information over the whole first Brillouin zone. Namely, the change across the phase boundary is much easier to elucidate, and the relation between the topological number and the helical edge modes is rather transparent. This work concerns local features in  $\vec{k}$  space, and is complementary to Refs. 5 and 26, which treats global topological structure in  $\vec{k}$  space. We ignore interaction and disorder effect in this paper, since the robustness of the system is inferred from the topological stability.

## II. GAP CLOSING AT THE PHASE TRANSITION

Since the phase transition necessarily accompanies closing of the gap,<sup>5,9,10</sup> we commence with an analysis of generic gap-closing in a two-dimensional (2D) gapped spin-1/2  $T$ -symmetric system with spin-orbit interaction. A Hamiltonian matrix for Bloch wavefunctions can be written in a block form

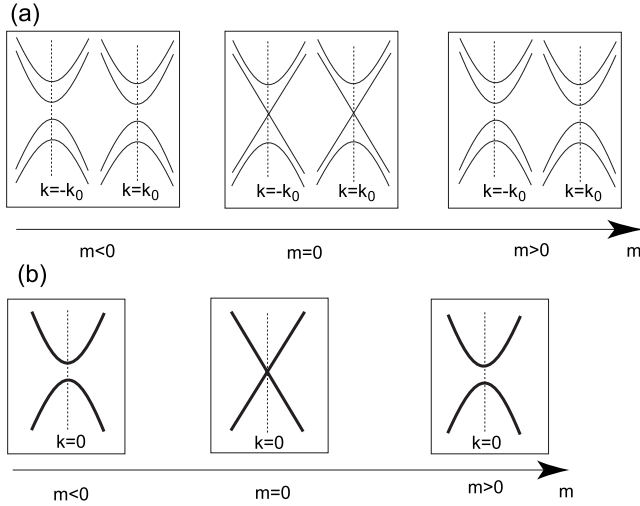


FIG. 1. Generic gap closing for (a) inversion-asymmetric and (b) inversion-symmetric cases. In case (b) all the states are doubly degenerate by Kramers theorem.

$$H(\vec{k}) = \begin{pmatrix} h_{\uparrow\uparrow}(\vec{k}) & h_{\uparrow\downarrow}(\vec{k}) \\ h_{\downarrow\uparrow}(\vec{k}) & h_{\downarrow\downarrow}(\vec{k}) \end{pmatrix}. \quad (1)$$

The dimension of the matrix  $h_{\sigma\sigma'}(\vec{k})$  depends on systems considered; nevertheless, in order to describe the phase transition, it is sufficient to restrict the dimension of the matrices  $h_{\sigma\sigma'}(\vec{k})$  to be one or two, as we will see later. To investigate the topological order of the Hamiltonian, its spectrum is assumed to have a gap, within which the Fermi energy lies. The  $T$  symmetry is represented by the operator  $\Theta = i\sigma_y K$  ( $\sigma_{x,y,z}$  are Pauli matrices and  $K$  stands for complex conjugation). For  $H(\vec{k})$  it implies

$$H(\vec{k}) = \sigma_y H^T(-\vec{k}) \sigma_y \quad (2)$$

or, equivalently,  $h_{\uparrow\uparrow}(\vec{k}) = h_{\downarrow\downarrow}^T(-\vec{k})$  and  $h_{\uparrow\downarrow}(\vec{k}) = -h_{\downarrow\uparrow}^T(-\vec{k})$ . This, in turn, results in a degeneracy between states at  $\vec{k}$  and  $-\vec{k}$ , forming Kramers pairs.

Tuning some parameters in the Hamiltonian may drive a transition, where the gap closes and degeneracies between the valence and the conduction bands occur at certain wave vectors  $\vec{k} = (k_x, k_y)$ . To pursue the phase transition, we will focus on “generic” gap closing achieved by tuning a single parameter  $m$ . (For mere convenience, the critical value of  $m$  for which a generic gap closing occurs is chosen as  $m=0$ .) Nongeneric gap closing achieved by tuning several parameters are excluded in our analysis. This is because such kind of gap closing can be circumvented by small perturbation, meaning that it cannot be associated with a phase transition. As we show below, generic gap closings are classified into two cases shown schematically in Figs. 1(a) and 1(b) (depending on symmetry under parity). We note that while we have not made any assumption on the  $Z_2$  topological number, both cases (a) and (b) turn out to encode quantum phase transitions between the QSH and the SHI phases. Among the known models describing this kind of phase transition, the Kane-Mele model on the honeycomb lattice<sup>5</sup> falls within

class (a) while the HgTe quantum well model<sup>18</sup> belongs to class (b).

The QSH-SHI phase transitions pertaining to Figs. 1(a) and 1(b) are not so trivial as it might look. In general, energy levels repel each other, thereby the valence and the conduction bands do not touch when the number of tuned parameters is not large enough. The number of tuned parameters to achieve degeneracy, called the codimension, is sensitive to the symmetry and the dimension of the system considered. For example, in three dimensions the gap closing type (a) in Fig. 1 does not occur.<sup>19</sup>

Consider now a spatial inversion ( $I$ ) symmetry which plays an important role in addition to  $T$  symmetry. The former requires the relation  $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\alpha}(-\vec{k})$ , while the latter implies  $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\bar{\alpha}}(-\vec{k})$ , where  $\varepsilon_{n\alpha}(\vec{k})$  is the energy of band  $n$  with pseudospin  $\alpha$ , and  $\bar{\alpha}$  is the pseudospin opposite to  $\alpha$ .<sup>20</sup> If both symmetries are respected,  $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\bar{\alpha}}(\vec{k})$  and there is a Kramers double degeneracy at each  $\vec{k}$ . If  $I$  symmetry is broken, double degeneracy occurs at points  $\vec{k} = -\vec{k} + \vec{G}$ , i.e.,  $\vec{k} = \vec{k}_i \equiv \vec{G}/2$ , where  $\vec{G}$  is a reciprocal lattice vector; no double degeneracy occurs at other points (unless an additional symmetry is present). The  $I$ -asymmetric and  $I$ -symmetric cases are therefore considered separately below.

### A. Inversion asymmetric systems

In this case, when  $\vec{k} \neq -\vec{k} + \vec{G}$ , each band is nondegenerate, and the gap between two bands can close at some points  $\vec{k}$ . At the gap-closing point, one valence band and one conduction band become degenerate. The codimension is 3.<sup>21</sup> This codimension 3 is equal to the number of parameters involved, that is,  $k_x$ ,  $k_y$ , and  $m$ . Thus the gap can close at some  $\vec{k}$  when the parameter  $m$  is tuned to a critical value.

On the other hand, when  $\vec{k} = -\vec{k} + \vec{G}$ , the band is doubly degenerate, and the codimension is 5,<sup>22,23</sup> exceeding the number of tunable parameters which is 1 (that is,  $m$ ). Thus, generic gap closing cannot occur at  $\vec{k} = \vec{G}/2$ .<sup>24</sup>

We thus focus on the case  $\vec{k} \neq \vec{G}/2$ . Near the gap-closing point  $\vec{k} = \vec{k}_0 (\neq \vec{G}/2)$ , the system’s Hamiltonian corresponds to massive two-component fermion, and can be expressed as  $\mathcal{H} = m\sigma_z + (k_x - k_{0x})\sigma_x + (k_y - k_{0y})\sigma_y$  (after unitary and scale transformations).  $T$  symmetry requires that the gap closes simultaneously at  $\vec{k}_0$  and  $-\vec{k}_0$  as depicted in Fig. 1(a), and that the masses at  $\vec{k} = \pm\vec{k}_0$  have opposite signs. In the honeycomb-lattice model for QSH (Refs. 4 and 5) the gap closes at the  $K, K'$  points; Hence it reduces to the present scheme without  $I$  symmetry.

### B. Inversion symmetric systems

In this case, the energies are doubly degenerate at each  $\vec{k}$ . At the phase transition, the gap between the two doubly degenerate bands closes. Hence, we consider  $4 \times 4$  Hamiltonian matrix  $H(\vec{k})$  [ $h_{\alpha\beta}(\vec{k})$  in Eq. (1) are  $2 \times 2$ ]. The  $I$  symmetry is imposed as

$$H(-\vec{k}) = PH(\vec{k})P^{-1}, \quad u(-\vec{k}) = Pu(\vec{k}), \quad (3)$$

where  $P$  is a unitary matrix independent of  $\vec{k}$ , and  $u(\vec{k})$  is the periodic part of the Bloch wave function  $\varphi_{\vec{k}}(\vec{r}) = u(\vec{k})e^{i\vec{k}\cdot\vec{r}}$ . As the inversion does not flip spin, this unitary matrix  $P$  should be block diagonal in spin space:

$$P = \begin{pmatrix} P_{\uparrow} & \\ & P_{\downarrow} \end{pmatrix}. \quad (4)$$

In fact, all cases reduce to a case  $P_{\uparrow} = P_{\downarrow} = \text{diag}(\eta_a, \eta_b)$  with  $\eta_a = \pm 1$ ,  $\eta_b = \pm 1$ , as can be shown directly by applying a unitary transformation.  $\eta_a$  and  $\eta_b$  represent the parity eigenvalues of the atomic orbitals.

Occurrence of gap closing turns out to be different for the cases (i)  $\eta_a = \eta_b$  and (ii)  $\eta_a = -\eta_b$ . The case (i)  $\eta_a = \eta_b = \pm 1$  is realized when the atomic orbitals  $a, b$  have the same parity, such as two  $s$ -like orbitals or two  $p$ -like orbitals. The ensuing constraints on the Hamiltonian are  $h_{\uparrow\uparrow} = h_{\downarrow\downarrow}^T$  is an even function of  $\vec{k}$ , and  $h_{\uparrow\downarrow} = h_{\downarrow\uparrow}^T$  is an antisymmetric matrix, even function in  $\vec{k}$ . In an explicit form, the generic Hamiltonian becomes

$$H(\vec{k}) = E_0(\vec{k}) + \sum_{i=1}^5 a_i(\vec{k})\Gamma_i, \quad (5)$$

where  $a_i$ 's and  $E_0$  are real even functions of  $\vec{k}$ .  $\Gamma_i$  are  $4 \times 4$  matrices given by  $\Gamma_1 = 1 \otimes \tau_x$ ,  $\Gamma_2 = \sigma_z \otimes \tau_y$ ,  $\Gamma_3 = 1 \otimes \tau_z$ ,  $\Gamma_4 = \sigma_y \otimes \tau_y$ , and  $\Gamma_5 = \sigma_x \otimes \tau_y$ , where  $\sigma_i$  and  $\tau_i$  are Pauli matrices acting on spin and orbital spaces, respectively. The eigenenergies are given by  $E_0 \pm \sqrt{\sum_{i=1}^5 a_i^2}$ . The gap closes when  $a_i(\vec{k}) = 0$  for  $i = 1, \dots, 5$ . It means that the codimension is 5, the same as in the case at  $\vec{k} = \vec{G}/2$  without  $I$  symmetry. Thus there are no solutions of  $k_x, k_y$ , and  $m$  which satisfy these five relations. The gap never closes in this case.

Next we consider the case  $\eta_a = -\eta_b = \pm 1$ , i.e.,  $P = \eta_a \tau_z = \pm \tau_z$ , where the two constituent atomic orbitals have different parity. The Hamiltonian reads

$$H(\vec{k}) = a_0(\vec{k}) + a_5(\vec{k})\Gamma'_5 + \sum_{i=1}^4 b^{(i)}(\vec{k})\Gamma'_i, \quad (6)$$

where  $a_0(\vec{k})$  and  $a_5(\vec{k})$  are even functions of  $\vec{k}$  and  $b^{(i)}(\vec{k})$  are odd functions of  $\vec{k}$ . Here  $\Gamma'_i$  are  $4 \times 4$  matrices given by  $\Gamma'_1 = \sigma_z \otimes \tau_x$ ,  $\Gamma'_2 = 1 \otimes \tau_y$ ,  $\Gamma'_3 = \sigma_x \otimes \tau_x$ ,  $\Gamma'_4 = \sigma_y \otimes \tau_x$ , and  $\Gamma'_5 = 1 \otimes \tau_z$ . In this case the gap closes only when five equations  $a_5(\vec{k}) = 0$ ,  $b^{(i)}(\vec{k}) = 0$  are satisfied. For a generic point  $\vec{k}$  with  $\vec{k} \neq \vec{G}/2$ , these five equations cannot be satisfied simultaneously, through a change of a single parameter.<sup>25</sup> On the other hand, at the high-symmetry points  $\vec{k} = \vec{k}_i = \vec{G}/2$ , the situation is different. At these points the odd functions  $b^{(i)}(\vec{k})$  vanish identically, and one has only to tune  $a_5(\vec{k})$  to be zero. Thus, the gap closes by fine-tuning a single parameter. To be more specific, we take  $\vec{k} = 0$  as an example, and write down the Hamiltonian explicitly. Extension to other  $\vec{k} = \vec{G}/2$  points is straightforward. The Hamiltonian is expanded to linear order in  $\vec{k}$  as

$$H(\vec{k}) \sim E_0 + m\Gamma'_5 + \sum_{i=1}^4 (\vec{\beta}^{(i)} \cdot \vec{k})\Gamma'_i, \quad (7)$$

where  $E_0$  and  $m$  are constants and  $\vec{\beta}^{(i)}$  ( $i = 1, \dots, 4$ ) are two-dimensional real constant vectors. Further simplification is obtained after judicious unitary transformations. The Hamiltonian finally acquires the block-diagonal form

$$H(\vec{k}) = E_0 + \begin{pmatrix} m & z_- & & \\ z_+ & -m & & \\ & & m & -z_+ \\ & & -z_- & -m \end{pmatrix}, \quad (8)$$

where  $z_{\pm} = b_1 k_x + b_3 k_y \pm i b_2 k_y$ , with real constants  $b_1, b_2$  and  $b_3$ . Note that in materials with high crystallographic symmetry (e.g., tetragonal), one has  $b_1 = b_2$  and  $b_3 = 0$ , leading to  $z_{\pm} \propto k_x \pm i k_y$ . We have thus demonstrated a feature: The Hamiltonian of a generic system with spin-orbit coupling obeying  $T$  and  $I$  symmetries decouples, after an appropriate choice of basis, into a pair of Hamiltonians describing two-component fermions with opposite sign of the corresponding mass terms. (Such decoupling is expected in the special case where  $s_z$  is a good quantum number, since the system describes two copies of a quantum Hall system). Experimental consequences are immediate as the Hamiltonian (8) is equivalent to the one suggested for the HgTe quantum well in Ref. 18 (based on phenomenological arguments). Gap closing at  $\vec{k} = 0$  when the parameter  $m$  is tuned to zero is now obvious, since the eigenenergies are  $E = E_0 \pm \sqrt{m^2 + z_+ z_-}$ . The inversion matrix in this basis is written as  $\eta_a \otimes \tau_z = \eta_a \text{diag}(1, -1, 1, -1)$ .

Summing up to this point, we discussed generic types of gap closing in time-reversal invariant systems, achieved by tuning a single parameter. Taking  $I$ -symmetry into consideration, two types of gap-closing scenarios have been found: (a) simultaneous gap closing at  $\vec{k} = \pm \vec{k}_0 \neq \vec{G}/2$  occur in systems without  $I$  symmetry and (b) gap closing between two Kramers-degenerate bands (i.e., four bands) at  $\vec{k} = \vec{G}/2$  occur in systems with  $I$  symmetry (see Fig. 1). Due to the level repulsion, the gap-closing by tuning a single parameter occurs only in limited cases. We will see in the subsequent discussion that these cases of gap closing exactly coincides with the phase transition between the QSH and the insulating phases. In this sense our theory characterizes the QSH phase from the local features in  $\vec{k}$  space.

### C. Change of the $Z_2$ topological number at the gap-closing point

Now we focus on the change of  $Z_2$  topological number at the gap closing, assuming that except for the gap closing ( $m=0$ ) the bands are fully gapped. Hence, both phases at  $m > 0$  and  $m < 0$  are band insulators, and have well-defined  $Z_2$  topological numbers. For the  $I$  symmetric case (a), the homotopy characterization in Ref. 26 is applicable; for the lower band at the critical value  $m=0$ , there is one vortex at  $\vec{k}_0$  and one antivortex at  $-\vec{k}_0$ . Thus, when the parameter  $m$  is tuned across  $m=0$ , the Chern number for the whole con-

tracted surface<sup>26</sup> changes by 1. Thus, the  $Z_2$  topological numbers are different by 1 for the  $m > 0$  and the  $m < 0$  sides. One of the phases is the QSH phase, while the other is the SHI. For the  $I$ -symmetric case (b), Fu and Kane<sup>13</sup> developed a simple method to calculate the  $Z_2$  topological number  $\Delta$  as

$$(-1)^\Delta = \prod_{i=1}^4 \prod_{m=1}^N \xi_{2m}(\vec{k}_i), \quad (9)$$

where  $\vec{k}_i$  are the four high-symmetry points satisfying  $\vec{k} = \vec{G}/2$ ,  $\xi_{2m}(k_i)$  is the parity eigenvalue at each of these points, and  $N$  is the number of Kramers pairs below  $E_F$ . In the present case the gap at  $\vec{k}=0$  collapses when  $m=0$ . Hence only the parity eigenvalue at  $\vec{k}=0$  can change at the phase transition. Since the inversion matrix is given by  $P = \eta_a \otimes \tau_z = \eta_a \sigma_0 \otimes \tau_z$ , the parity eigenvalues are  $-\eta_a (= \eta_b)$  and  $+\eta_a$  for the lower-band states at  $m > 0$  and  $m < 0$ , respectively. Hence, the parity eigenvalue changes sign, and the  $Z_2$  topological number  $\Delta$  changes by 1. Thus, on the two sides of the band touching,  $m > 0$  and  $m < 0$ , one of the phases is the QSH phase, while the other one is the simple insulator (SHI) phase.

### III. HELICAL EDGE STATES

Let us regard the usual insulating phase as our vacuum, so that the domain wall between the QSH phase and the insulating phase is the edge of the sample. Such a domain wall is described by a spatially dependent mass parameter  $m(x)$  satisfying  $m(\pm\infty) = \pm m_0$ , i.e.,

$$m = \begin{cases} m_0 & x \gg 0, \\ -m_0 & x \ll 0. \end{cases} \quad (10)$$

We do not specify the detail of the crossover between  $m_0$  and  $-m_0$ , because it is not important for the subsequent discussions. For Fig. 1(a), one can consider the Weyl fermions at  $\vec{k} = \pm \vec{k}_0$  separately. Masses of these Weyl fermions change sign at  $m=0$ ; hence they yield the edge states localized at the domain wall, as explained in Ref. 27. Because the Weyl fermions at  $\vec{k} = \pm \vec{k}_0$  are related to each other by time-reversal symmetry, the two edge states form a Kramers pair.

For Fig. 1(b) with a domain wall (10), we follow the discussion in Ref. 27 to show that such domain wall between phases with different  $Z_2$  topological number possesses one Kramers pair of edge states at the boundary. In this case we consider

$$\tilde{H}(k_y) = E_0 + \begin{pmatrix} m & -ib_1\partial_x + (b_3 - ib_2)k_y & & \\ -ib_1\partial_x + (b_3 + ib_2)k_y & -m & & \\ & & m & ib_1\partial_x - (b_3 + ib_2)k_y \\ & & ib_1\partial_x - (b_3 - ib_2)k_y & -m \end{pmatrix}. \quad (11)$$

To calculate the eigenstates it is convenient to perform unitary transformation as

$$\begin{aligned} H'(k_y) &= Q^\dagger \tilde{H}(\vec{k}) Q \\ &= E_0 + \begin{pmatrix} b_2k_y & m - b_1\partial_x & & \\ m + b_1\partial_x & -b_2k_y & & \\ & & -b_2k_y & m - b_1\partial_x \\ & & m + b_1\partial_x & b_2k_y \end{pmatrix}, \end{aligned} \quad (12)$$

where

$$Q = e^{-ib_3k_y x/b_1} \begin{pmatrix} 1 & 1 & & \\ i & -i & & \\ & & -i & -i \\ & & -1 & 1 \end{pmatrix}. \quad (13)$$

We omit the term  $E_0$  henceforth, since it does not affect the subsequent discussions. The eigenvalue problem reads as  $H'(k_y)u_{k_y}(x) = E(k_y)u_{k_y}(x)$ .

Because Eq. (12) is block-diagonal, we first solve the eigenvalue problem for the first two components of  $u_{k_y}$ , i.e., we put  $u_{k_y} = (u_1, u_2, 0, 0)^t$ . We get

$$(E - b_2k_y)u_1 = Du_2, \quad (14)$$

$$(E + b_2k_y)u_2 = D^\dagger u_1, \quad (15)$$

where  $D = m - b_1\frac{\partial}{\partial x}$ ,  $D^\dagger = m + b_1\frac{\partial}{\partial x}$ . They yield eigenequations for  $u_1$  and  $u_2$ , respectively,

$$DD^\dagger u_1 = (E^2 - b_2^2k_y^2)u_1, \quad (16)$$

$$D^\dagger D u_2 = (E^2 - b_2^2k_y^2)u_2. \quad (17)$$

When we solve Eq. (16) for  $u_1$ , one can calculate  $u_2$  from Eq. (15). As Eq. (16) is invariant under  $E \rightarrow -E$ , it seems that the solutions for  $E$  and  $-E$  are always obtained simultaneously, namely there is a spectral symmetry between  $E \leftrightarrow -E$ . Nevertheless, it does not apply if  $E = -b_2k_y$ , where Eq. (15) cannot be solved for  $u_2$ . A similar situation occurs for  $E = b_2k_y$ . Thus exceptions at  $E = \pm b_2k_y$  occur in the following way. For  $u_1 (\neq 0)$  which satisfies  $D^\dagger u_1 = 0$ , we get  $E = b_2k_y$  and  $u_2 = 0$

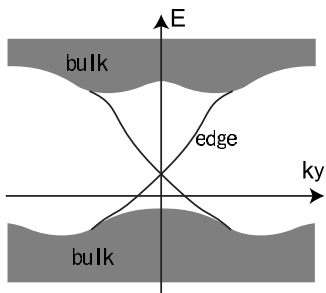


FIG. 2. Schematic dispersion curves for the model (11). Kramers theorem guarantees that the crossing of two edge states occur at  $k_y=0$ .

from Eqs. (14) and (15), whereas there is no solution with  $E=-b_2k_y$ . In the same token, for  $u_2$  which satisfies  $Du_2=0$ , we get  $E=-b_2k_y$  from Eq. (14), whereas there is no solution with  $E=b_2k_y$ . Hence the spectral asymmetry is related to the kernels for  $D$  and  $D^\dagger$ . For simplicity we take  $b_1>0$  henceforth, while the other case of  $b_1<0$  can be studied in a similar way. For the domain wall (10), the solution of  $D^\dagger u_1=0$  gives

$$u_1 \propto \exp\left(-b_1^{-1} \int^x m(s) ds\right) \quad (18)$$

and  $E=b_2k_y$ , while  $Du_2=0$  has no normalizable solution. Thus the energy dispersion in  $k_y$  direction has a branch  $E=b_2k_y$ , which crosses the Fermi energy  $E\sim 0$ . This state is gapless, localized near  $x=0$ .

So far we have solved the eigenequation for the first two components. The lower two components of the wavefunction  $u$  is obtained from above by time-reversal operation [ $\Theta u(k_y)=i\sigma_2 u(-k_y)^*$ ]. Therefore, the abovementioned edge state with  $E=b_2k_y$  has a Kramers partner with  $E=-b_2k_y$ . The whole dispersion is shown in Fig. 2. Thus we have shown that the Kramers pair of edge states exists at the boundary between the two phases. They cross at  $k_y=0$ , as is guaranteed by the Kramers theorem.

#### IV. CONCLUSIONS

A general framework is established for classifying phase transitions between the quantum spin Hall and the insulator phases. For inversion-asymmetric systems, the phase transition accompanies a gap closing at  $\vec{k}=\pm\vec{k}_0$  which is not at the high-symmetry points. For inversion-symmetric systems, the gap closes only at  $\vec{k}=\vec{G}/2$  where  $\vec{G}$  is a reciprocal vector. The models in Refs. 4, 5, and 18 exhibiting phase transition between the two phases are special cases of this general classification framework.

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