Chern number of thin films of the topological insulator Bi_2Se_3

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In thin films of Bi_2Se_3 , the isospin sectors have nontrivial topological properties, which are conventionally characterized by the Z_2 index. The generalized isospin Chern number [E. Prodan, *Phys. Rev. B* **80**, 125327 (2009)] is calculated in the general case where the structural inversion symmetry is broken and the isospin operator $\hat{\tau}_z$ is not conserved. The analytical formalism obtained reveals clearly the connection between the isospin Chern number and the Z_2 index. We further demonstrate that the topological characterization based on the isospin Chern number fully agrees with the characteristic spectrum of the edge states in different regimes.

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I. INTRODUCTION

The quantum spin-Hall effect (QSHE) is a state of matter originating from spin-orbit coupling, which preserves the time-reversal symmetry. In the QSHE state, the material possesses a bulk energy gap and allows for dissipationless charge transport through gapless spin-filtered edge states. The earliest proposal of the existence of the QSHE was due to Kane and Mele,¹ and Bernevig and Zhang.² The Kane and Mele model¹ is essentially two copies of the Haldane model defined on a two-dimensional (2D) honeycomb lattice for integer quantum Hall effect (IQHE) without Landau levels.³ In the Kane and Mele model, the spin up and spin-down electrons exhibit opposite Hall conductivities $\pm e^2/h$ due to the spin-orbit coupling, so that the total charge Hall conductivity vanishes but the spin Hall conductivity is 2, in units of spin Hall conductance quantum $e/4\pi$. The Bernevig and Zhang model² considers an intricate 2D strain architectural structure, where the spin-orbit coupling of the electrons plays the role of a spin-dependent magnetic field. The QSHE state is robust against weak disorder scattering,⁴ and has recently been observed experimentally in HgTe.^{5,6} The QSHE systems are an example of topologically ordered states, which are also referred as topological insulators. It has been argued that the nontrivial topology of the bulk energy band can be characterized by a Z_2 index⁷ or a spin Chern number.⁸

Topological insulators in three dimensions^{9,10} have attracted much attention in recent years. Three-dimensional (3D) topological insulators have gapless spin-textured surface states in the bulk band gap, which are protected by time-reversal symmetry. The theoretical prediction^{9,10} was later confirmed experimentally in bismuth antimony alloys, and in Bi_2Se_3 and Bi_2Te_3 compounds by using some different experimental technologies.^{11–16} In particular, Bi_2Se_3 and Bi_2Te_3 have bulk energy gaps as large as 0.3 eV, with surface states consisting of a single Dirac cone, in contrast to the paired Dirac cones in graphene. The metallic nature of the surface states is ensured by the nontrivial Berry phase at the Dirac point, which cannot be eliminated by scattering of weak nonmagnetic disorder. The metallic surface states may have application in low-dissipation quantum computing, electronic, or spintronic devices.

In thin films of 3D topological insulators, the surface states on the two surfaces hybridize to create a gap in the

energy spectrum. The gap displays an oscillating exponential decay with film thickness.^{17,18} Depending on the thickness and other material parameters, the system may become a topologically trivial or nontrivial insulator.¹⁸ For the purpose of practical applications, it is important to study the related phase transitions and the surface state properties in different phases. By using a continuum model for the surface states, Shan *et al.*¹⁸ calculated the isospin-dependent Hall conductivity and Chern number in the presence of structural inversion symmetry, where the isospin $\hat{\tau}_z$ is a conserved quantity. Here, by isospin we mean bonding and antibonding of the electron states at the two surfaces. When the structural inversion symmetry is broken and $\hat{\tau}_z$ is no longer conserved, they turned to the Z_2 index, whereby the topologically trivial and nontrivial phases were identified.

The spin Chern number was proposed to characterize the topological order of the bulk electron wave functions in the 2D QSHE models,⁸ which is a generalization of the Chern number that was used to describe the topological order in the IQHE systems.¹⁹ The spin Chern number was originally defined for finite-size systems by introducing spin-dependent boundary phases.⁸ Recently, Prodan²⁰ established a new formalism for the spin Chern number at the thermal dynamic limit based upon the noncommutative Chern number theory²¹ without using spin-dependent boundary phases. In particular, the author proved that the spin Chern number is a true topological invariant protected by the bulk energy gap and the spin spectrum gap, rather than any symmetries. As long as these two gaps do not close, the spin Chern number remains unchangeable under smooth deformations of the system Hamiltonian, including those breaking time-reversal symmetry. While some numerical computations^{8,22,23} have been done before, an explicit analytical calculation of the spin Chern number will be very useful for understanding the physical implications of this topological invariant, which, however, has not been performed so far.

In this paper, with thin films of 3D topological insulator Bi_2Se_3 as an example of topologically nontrivial systems, we calculate explicitly the isospin Chern number by using the continuum model.¹⁸ Our result is valid in the general case where the structural inversion symmetry is broken and $\hat{\tau}_z$ is not conserved, which recovers the result obtained by Shan *et al.*¹⁸ if the structural inversion symmetry is restored. We ob-

serve a clear connection between the isospin Chern number and the Z_2 index, which agree with each other in all quantum phases of the systems. The calculated spectrum of the edge states in different regimes is also consistent with the Chern number characterization.

In the next section, we introduce the model Hamiltonian, and study its energy spectrum and wave functions. In Sec. III, analytical calculation of the isospin Chern number is carried out. In Sec. IV, a comparison between the isospin Chern number and the Z_2 index is made. In Sec. V, the edge state spectrum in different regimes is calculated by constructing a tight-binding model. The final section is a summary.

II. MODEL HAMILTONIAN

We consider an ultrathin film of Bi_2Se_3 grown along the z direction of thickness L . The two surfaces are assumed to locate at $z = \pm L/2$. In the compound Bi_2Se_3 , the low-energy physics of electrons is mainly controlled by electron states near the Γ point. The relevant outshell states are the four hybridized Bi and Se p_z orbitals, denoted as $|P1_z^+, \uparrow\rangle$, $|P2_z^-, \uparrow\rangle$, $|P1_z^+, \downarrow\rangle$, and $|P2_z^-, \downarrow\rangle$, where $+$ ($-$) represents states of even (odd) parity, and $\uparrow$ ($\downarrow$) stands for up (down) spin. The kets represent the four-component spinor wave functions. By following Zhang *et al.*,¹² the 4×4 low-energy effective Hamiltonian for Bi_2Se_3 on the basis of the four p_z orbitals is written as

$$H_{3D}(\mathbf{k}) = \begin{pmatrix} \varepsilon_k + M_k & -iA_1\partial_z & 0 & A_2k_- \\ -iA_1\partial_z & \varepsilon_k - M_k & A_2k_- & 0 \\ 0 & A_2k_+ & \varepsilon_k + M_k & iA_1\partial_z \\ A_2k_+ & 0 & iA_1\partial_z & \varepsilon_k - M_k \end{pmatrix}, \quad (1)$$

where $\hbar$ is taken to be unity, $k_{\pm} = k_x \pm ik_y$, $\varepsilon_k = C - D_1\partial_z^2 + D_2k^2$, and $M_k = M + B_1\partial_z^2 - B_2k^2$ with $k^2 = k_x^2 + k_y^2$. The parameters in the model have been determined by fitting the Bi_2Se_3 band structure from first-principles calculation¹² $C = -6.8 \times 10^{-3}$ eV, $M = 0.28$ eV, $A_1 = 2.2$ eV $\text{\AA}^2$, $A_2 = 4.1$ eV $\text{\AA}^2$, $B_1 = 10$ eV $\text{\AA}^2$, $B_2 = 56.6$ eV $\text{\AA}^2$, $D_1 = 1.3$ eV $\text{\AA}^2$, and $D_2 = 19.6$ eV $\text{\AA}^2$. The bulk states of the above Hamiltonian usually have a finite energy gap around the Fermi energy, and surface states exist within the energy gap.

To derive the effective Hamiltonian of the surface states, one can first solve the eigenstates of the Hamiltonian $H_{3D}(\mathbf{k})$ at the Γ point ($k_x = k_y = 0$), which are denoted as $\Phi_{\sigma\tau}(z)$. Here, $\sigma = \uparrow$ ($\downarrow$) represents the electron spin, and $\tau = \pm$ stands for the bonding and antibonding of the electron states at the two surfaces, which will be called “isospin.” The effective Hamiltonian is then obtained by expanding the Hamiltonian $H_{3D}(\mathbf{k})$ in Eq. (1) with the four surface states $\Phi_{\sigma\tau}(z)$ at the Γ point as a basis¹⁸

$$H(k) = E_0 - Dk^2 + \left(\frac{\Delta}{2} - Bk^2\right)\hat{\tau}_z\hat{\sigma}_z + v_F(k_y\hat{\sigma}_x - k_x\hat{\sigma}_y) + \gamma U\hat{\tau}_x, \quad (2)$$

where $\hat{\sigma}_\alpha$ and $\hat{\tau}_\alpha$ with $\alpha = x, y, z$ are the Pauli matrices related to electron spin and isospin. We have assumed that a gate voltage is applied between the two surfaces of the

FIG. 1. (Color online) The parameters in the effective Hamiltonian Eq. (2), calculated as functions of film thickness.

Bi_2Se_3 film, so that a static potential $-Uz/L$ is generated across the film, resulting in the $\gamma U\hat{\tau}_x$ term, where $\gamma = \int_{-L/2}^{L/2} \Phi_{\sigma+}^\dagger(z)(-z/L)\Phi_{\sigma-}(z)dz = \int_{-L/2}^{L/2} \Phi_{\sigma-}^\dagger(z)(-z/L)\Phi_{\sigma+}(z)dz$. The gate voltage breaks the structural inversion symmetry, and couples states with same spin and opposite isospin. In Fig. 1, four parameters B , D , Δ , and γ that are most relevant to our further discussions are plotted.

By direct diagonalization of the Hamiltonian Eq. (2), the eigenenergies are obtained as

$$E_{1\pm} = E_0 - Dk^2 \pm \sqrt{\left(\frac{\Delta}{2} - Bk^2\right)^2 + (\gamma U + v_F k)^2}, \quad (3)$$

$$E_{2\pm} = E_0 - Dk^2 \pm \sqrt{\left(\frac{\Delta}{2} - Bk^2\right)^2 + (\gamma U - v_F k)^2}, \quad (4)$$

where $+$ ($-$) stands for the conduction (valence) bands. The energy band is twofold degenerated at $\gamma U = 0$, and the degeneracy is lifted when γU is nonzero. The γU term plays a role similar to the Rashba spin-orbit coupling in the 2D electron systems. The wave functions of the two valence bands are given by

$$\varphi(k) = A_+ \begin{bmatrix} if_+(k)e^{-i\theta_k} \\ -v_F k - \gamma U \\ -i(v_F k + \gamma U)e^{-i\theta_k} \\ f_+(k) \end{bmatrix}, \quad (5)$$

$$\chi(k) = A_- \begin{bmatrix} -if_-(k)e^{-i\theta_k} \\ v_F k - \gamma U \\ -i(v_F k - \gamma U)e^{-i\theta_k} \\ f_-(k) \end{bmatrix} \quad (6)$$

with

FIG. 2. (Color online) Energy spectrum of surface states for some values of film thickness and gate voltage (a) $L=22$ Å, $U=0.2$ eV, (b) $L=28$ Å, $U=0.2$ eV, (c) $L=28$ Å, $U=0.5045$ eV, and (d) $L=28$ Å, $U=0.8$ eV.

$$f_{\pm}(k) = Bk^2 - \frac{\Delta}{2} + \sqrt{\left(Bk^2 - \frac{\Delta}{2}\right)^2 + (\gamma U \pm v_F k)^2}. \quad (7)$$

θ_k is the polar angle of the momentum $\mathbf{k}=(k_x, k_y)$ and $A_{\pm} = 1/\sqrt{2[f_{\pm}^2(k) + (v_F k \pm \gamma U)^2]}$ are normalization constants.

When $B^2 > D^2$, the valence band is inverted. Under this condition, if Δ and B have different signs, say, $\Delta/B < 0$, an energy gap always exists between the conduction and valence bands. If Δ and B have the same sign, i.e., $\Delta/B > 0$, an energy gap opens at small $|U|$. When $|U|$ reaches a critical value $U_0 = \frac{v_F}{\gamma} \sqrt{\frac{\Delta}{2B}}$, the energy gap closes. With further increasing $|U|$, the gap reopens. In Fig. 2, the calculated energy spectrum at two selected film thicknesses is plotted for some different values of U . Figure 2(a) ($L=22$ Å) corresponds to the case $\Delta/B < 0$, a gap exists in the energy spectrum. Figures 2(b)–2(d) ($L=28$ Å) correspond to the case $\Delta/B > 0$. We note that at this film thickness, the critical gate voltage is $U_0=0.5045$ eV. From the figures, we can see that a gap exists for (b) $|U| < U_0$, closes at (c) $|U|=U_0$, and then reopens for (d) $|U| > U_0$.

III. ISOSPIN CHERN NUMBER

If the gate voltage vanishes ($U=0$), the Hamiltonian is block diagonal for the isospin, and $\hat{\tau}_z$ becomes a conserved quantity. Shan *et al.*¹⁸ found that the Hall conductivity of the τ subband $\sigma_{xy} = C\tau e^2/h$, where $C_{\tau} = -\tau[\text{sgn}(\Delta) + \text{sgn}(B)]/2$ is the Chern number of the subband with $\text{sgn}(\dots)$ the usual sign function. When Δ and B have the same sign, the Chern number is quantized to a nonzero integer values $+1$ or -1 . This indicates that the system is in a topologically nontrivial phase (QSHE phase). When $U \neq 0$, calculation of the τ -dependent Chern number becomes tricky, as $\hat{\tau}_z$ is no longer a conserved quantity. However, in the following calculations, we will show that the isospin Chern number can be well defined, to characterize the whole QSHE phase, even when $\hat{\tau}_z$ is not conserved.

FIG. 3. (Color online) $\eta(k)t(k)$ for various values of gate voltage U at (a) $L=22$ Å and (b) $L=28$ Å. $\lambda_{\pm}(k)$ for (c) $L=22$ Å, $U=0.2$ eV, (d) $L=28$ Å, $U=0.2$ eV, and (e) $L=28$ Å, $U=0.8$ eV.

The definition of the isospin Chern number generally relies on a smooth decomposition of the occupied valence band into two sectors through diagonalization of the operator $\hat{\tau}_z$ in the valence band.²⁰ Since $\hat{\tau}_z$ commutes with momentum, the decomposition can be done for each $\mathbf{k}$ separately. By expressing $\hat{\tau}_z$ as a 2×2 matrix on the basis of $\varphi(k)$ and $\chi(k)$, we obtain for the eigenvalues of $\hat{\tau}_z$ as $\lambda(k) = \lambda_{\pm}(k) \equiv \pm |t(k)|$, where

$$t(k) = -2A_+A_-[f_+f_- + (v_F)^2k^2 - (\gamma U)^2]. \quad (8)$$

The corresponding eigenfunctions of $\hat{\tau}_z$ are

$$\psi_{\pm}(k) = \frac{1}{\sqrt{2}}[\varphi(k, \theta_k) \pm \xi_k \chi(k, \theta_k)], \quad (9)$$

where $\xi_k = -\text{sgn}[t(k)]$. Clearly, the spectrum of $\hat{\tau}_z$ consists of two branches, which can be used to decompose the valence band into two isospin sectors.

Before proceeding to the calculation of the Chern number, we shall study first the properties of the spectrum of $\hat{\tau}_z$. We notice that $t(k)$ is discontinuous as a function of k . For convenience of discussion, we define a continuous function $\eta(k)t(k)$, where $\eta(k) = \text{sgn}(k - k_0)$ with $k_0 = \frac{\gamma U}{v_F}$, if $B < 0$ and $|U| \geq U_0$, or $\Delta > 0$ and $|U| < U_0$, and $\eta(k)=1$ otherwise. Since $|\eta(k)|=1$, the eigenvalues of $\hat{\tau}_z$ can also be expressed in terms of $\eta(k)t(k)$ as $\lambda_{\pm}(k) = \pm |\eta(k)t(k)|$. For $\Delta/B < 0$, $\eta(k)t(k)$ is always negative for $k \in [0, \infty)$, suggesting that $\lambda_{\pm}(k)$ always has a gap around zero. For $\Delta/B > 0$, $\eta(k)t(k)$ is always negative if $|U| < U_0$, and hence $\lambda_{\pm}(k)$ always has a gap. However, if $|U| \geq U_0$, $\eta(k)t(k)$ crosses zero at $k=k_1 = \sqrt{\frac{\Delta}{2B}}$, indicating that $\lambda_+(k)$ and $\lambda_-(k)$ will touch each other at $k=k_1$. In Figs. 3(a) and 3(b), $\eta(k)t(k)$ at two selected film thicknesses $L=22$ Å and 28 Å as a function of k for some different values of U is plotted. For $L=22$ Å, where $\Delta/B < 0$, $\eta(k)t(k)$ is always negative for all values of U . For $L=28$ Å, where $\Delta/B > 0$, $\eta(k)t(k)$ is always negative for $|U| < U_0 (=0.5045$ eV), and crosses zero at $k=k_1$ for $|U| \geq U_0$. Figures 3(c)–3(e) illustrate the behavior of the spectrum $\lambda_{\pm}(k)$ of $\hat{\tau}_z$ in the three different regimes (c) $\Delta/B < 0$, (b)

FIG. 4. (Color online) Phase diagram of thin films of 3D topological insulator determined by the Chern numbers in the U versus L plane. (b) $P(k)$ as a function of k for $L=22$ Å, $U=0.2$ eV (red dashed line) and $L=28$ Å, $U=0.2$ eV (blue solid line).

$\Delta/B > 0$ and $|U| < U_0$, and (e) $\Delta/B > 0$ and $|U| > U_0$.

As long as the gap between the two branches $\lambda_{\pm}(k)$ of the $\hat{\tau}_z$ spectrum does not vanish, the electron states in the valence band are unambiguously decomposed into two sectors, namely, $\psi_+(k)$ and $\psi_-(k)$. One can define a Chern number²⁴ for each sector

$$C_{\pm} = \frac{1}{2\pi} \int d^2k F_{\pm}(k), \quad (10)$$

where $F_{\pm}(k) = i\hat{e}_z \cdot [\nabla_k \times \langle \psi_{\pm}(k) | \nabla_k | \psi_{\pm}(k) \rangle]$. It has been proved²⁰ that the Chern numbers of the two sectors are true topological invariants, which are robust against continuous deformations of the system Hamiltonian, including any symmetry-breaking perturbations.

By using the expression for the Laplace operator in the polar coordinate system $\nabla_k = \hat{e}_k \frac{\partial}{\partial k} + \hat{e}_{\theta_k} \frac{1}{k} \frac{\partial}{\partial \theta_k}$, it is straightforward to obtain $F_{\pm}(k) = \mp \frac{1}{2k} \frac{\partial}{\partial k} P(k)$, where

$$P(k) = 2A_+A_- \xi_k [f_+f_- - (v_F)^2 k^2 + (\gamma U)^2]. \quad (11)$$

Substituting these relations into Eq. (10), we obtain for the Chern numbers

$$C_{\pm} = \mp [P(\infty) - P(0)]. \quad (12)$$

Under the condition that the gap in the $\hat{\tau}_z$ spectrum does not vanish, namely, $\Delta/B < 0$, or $\Delta/B > 0$ and $|U| < U_0$,

$$\xi_k = \begin{cases} 1 & \Delta < 0 \\ \text{sgn}(k - k_0) & \Delta > 0 \end{cases} \quad (13)$$

and $P(k)$ is a continuous function of k . We have $P(0) = -\text{sgn}(\Delta)$ and $P(\infty) = \text{sgn}(B)$, so that the Chern number is

$$C_{\pm} = \mp \frac{1}{2} [\text{sgn}(\Delta) + \text{sgn}(B)]. \quad (14)$$

The Chern number is apparently an integer. This result is the same as the result obtained by Shan *et al.*¹⁸ However, our calculation proves it to be valid even when the structural inversion symmetry is broken, and $\hat{\tau}_z$ is no longer conserved.

Taking into account the condition $(B^2 - D^2) > 0$ for band inversion and the expression for the Chern number, Eq. (14), we determine a phase diagram for the topological insulator Bi_2Se_3 film, as plotted in Fig. 4(a). If the film thickness is smaller than a critical thickness about $L_0 = 25.1$ Å, the sys-

tem is an ordinary insulator, because $B < 0$ and $\Delta > 0$ such that $C_{\pm} = 0$. Between $L_0 = 25.1$ Å and about $L_1 = 32.3$ Å, the system is a topologically nontrivial QSHE insulator for $|U| < U_0$, where $B < 0$, $\Delta < 0$ and so $C_{\pm} = \pm 1$. The behavior of $P(k)$ as a function of k in the two regions is illustrated in Fig. 4(b). We recall that at $|U| = U_0$, the gap between the conduction and valence bands closes, and then reopens with further increasing $|U|$. Meanwhile, the spectrum gap of $\hat{\tau}_z$ between $\lambda_+(k)$ and $\lambda_-(k)$ vanishes at $|U| = U_0$ but does not reopen for $|U| > U_0$. This suggests that the electron states in the occupied valence band can no longer be decomposed unambiguously by using the operator $\hat{\tau}_z$ alone, giving rise to certain uncertainty in defining the Chern numbers. Such a region is shaded in the phase diagram, which will be revisited in next section. We mention that for $L > L_1$, $(B^2 - D^2) < 0$, the band inversion condition does not hold, and there will be no gap in the surface states.

IV. TOPOLOGICAL CHERN NUMBER VERSUS Z_2 INDEX

The Z_2 index⁷ can be obtained by counting the number of pairs of complex zeros of the *Pfaffian* of an antisymmetric matrix defined by the overlaps of time reversal, namely, $\tilde{P}(k) = \text{Pf}[A(\mathbf{k})]$ with $A_{ij}(\mathbf{k}) = \langle u_i(k) | \Theta | u_j(k) \rangle$. $\Theta = i\hat{\tau}_x \hat{\sigma}_y K$ is the time reversal operator with K the complex conjugate operator, and i, j runs over all the subbands below the Fermi surface, i.e., $\phi(k)$ and $\chi(k)$ for the present case. With some elegant analytical techniques, Shan *et al.*¹⁸ have obtained the expressions for $\tilde{P}(k)$. Surprisingly, in the regions where $\Delta/B < 0$ or $\Delta/B > 0$ and $|U| < U_0$, we find that their expression for $\tilde{P}(k)$ is exactly the same as $P(k)$ obtained in this paper $\tilde{P}(k) \equiv P(k)$, though the two expressions are derived by quite different approaches. The Z_2 classification focuses on the signs of $\tilde{P}(0)$ and $\tilde{P}(\infty)$. If $\tilde{P}(0)\tilde{P}(\infty) > 0$, $\tilde{P}(k)$ will have even pairs of zeros with k_x running from $-\infty$ to ∞ , which is considered to be topologically trivial. If $\tilde{P}(0)\tilde{P}(\infty) < 0$, $\tilde{P}(k)$ has odd pairs of zeros, corresponding to a topologically nontrivial state. On the other hand, the Chern number classification evaluates the difference between $P(\infty)$ and $P(0)$. Clearly, whenever the Z_2 index is nontrivial, the Chern number $C_{\pm} = \pm [P(\infty) - P(0)]$ must be nonzero. In general, the inverse proposition is not true.

Now we turn to the region where $\Delta/B > 0$ and $|U| > U_0$, where the Chern number has not been defined so far. In this region, the spectrum of $\hat{\tau}_z$ is gapless; the $\lambda_+(k)$ branch and $\lambda_-(k)$ branch touch each other at $k=k_1$, which brings some complexity into the definition of the Chern number. Assume that we start from $k=\infty$, and move along the $\lambda_-(k)$ branch to $k=k_1$. We then have two choices to reach $k=0$, through either of the two branches $\lambda_-(k)$ and $\lambda_+(k)$, which are indicated as paths 1 and 2 in Fig. 5(a). If we choose the electron states on path 1 as a sector and the reminder states as another sector, we can derive an expression for $P(k)$ that is the same as Eq. (11) with ξ_k still given by Eq. (13). However, this $P(k)$ is found not to be a continuous function of k in this region, as plotted in Fig. 5(b) as a dotted line. Clearly, $P(k)$ jumps at $k=k_1$. On the other hand, if we choose path 2, we find that $P(k)$ can still be written as Eq. (11) but ξ_k is given by

FIG. 5. (Color online) (a) $\lambda_{\pm}(k)$ and (b) $P(k)$ as functions of k , for $L=28$ Å, $U=0.8$ eV.

$$\xi_k = \begin{cases} \text{sgn}(k - k_0) & B < 0 \\ 1 & B > 0 \end{cases} \quad (15)$$

$P(k)$ obtained in this way is a continuous function of k , as shown in Fig. 5(b) as a solid line. To define the Chern number, it is reasonable to choose the continuous function of $P(k)$. Physically, the continuity of $P(k)$ with changing k reflects the smoothness of the decomposition of the valence band. It is easy to find that $P(\infty)=P(0)=\text{sgn}(B)$, so that $C_{\pm}=0$. Therefore, the system is an ordinary insulator in this region (shaded region in the phase diagram). Surprisingly, in the current region, our expression for $P(k)$, Eqs. (11) and (15), is consistent with the expression for $\tilde{P}(k)$ derived by Shan *et al.*¹⁸ as well.

V. EDGE STATES

In the QSHE phase, the Chern number $C_{\pm} = \pm 1$ indicates that there are a pair of edge modes counterpropagating at the open boundary of the film, which are isospin polarized. On the other hand, in the insulator regions, $C_{\pm}=0$ implies that no edge modes exist at the open boundary of the system. To simulate the edge state spectrum, we construct a tight-binding model, which recovers the continuum Hamiltonian Eq. (2) in the long-wavelength limit

$$H(k) = \left(E_0 + \frac{\Delta}{2} \hat{\sigma}_z \hat{\tau}_z \right) - \frac{2}{a_0^2} (D + B \hat{\sigma}_z \hat{\tau}_z) \times [2 - \cos(k_x a_0) - \cos(k_y a_0)] + \frac{v_F}{a_0} [\sin(k_y a_0) \hat{\sigma}_x - \sin(k_x a_0) \hat{\sigma}_y] + \gamma U \hat{\tau}_x, \quad (16)$$

where a_0 is the lattice constant of the underlying square lattice. We consider an infinitely long stripe geometry of a thin film of the 3D topological insulator running along the x direction with width $N_y a_0$. Open boundary conditions are imposed at the two edges of the stripe. The system has translational invariance along the x direction, so that the x component of the momentum k_x is a good quantum number, which can be utilized to simplify the calculation.

FIG. 6. (Color online) Energy spectrum of surface and edge states as a function of $k_x a_0$ calculated from the tight-binding model for some values of film thickness and gate voltage (a) $L=22$ Å, $U=0$ eV; (b) $L=28$ Å, $U=0$ eV; (c) $L=28$ Å, $U=0.2$ eV; and (d) $L=28$ Å, $U=0.8$ eV, where the lattice constant and stripe width are taken to be $a_0=\text{Å}$, and $N_y=1600$.

Figure 6 shows the low-energy spectrum for some different sets of parameters. Figure 6(a) corresponds to the $C_{\pm}=0$ region, from which we can see that there is no edge state mode in the energy gap of the surface states. Figures 6(b) and 6(c) correspond to the $C_{\pm} = \pm 1$ region, for $\gamma U=0$ and $\gamma U \neq 0$, respectively. In both cases, there exist two gapless edge state modes connecting up the conduction and valence bands. The existence of the edge state modes has its topological origin in the nonzero isospin Chern number. However, their gapless nature is not a consequence of the topology; it is due to the time-reversal symmetry. Figure 6(d) corresponds to the shaded region in the phase diagram, where no gapless edge state modes exist. The above results are fully consistent with the discussions based upon the isospin Chern number presented in previous sections.

VI. A SUMMARY

In this paper, we studied the topological invariant isospin Chern number for thin films of 3D topological insulator Bi_2Se_3 . We showed that the isospin Chern number can be used to describe the topologically trivial and nontrivial phases and the related quantum phase transition, in the general case where the structural inversion symmetry is broken and the isospin operator is not conserved. Clearly, for the system with time reversal symmetry that we studied, the isospin Chern number and the Z_2 index lead to equivalent identification of the quantum phases. The edge state spectrum calculated for an infinitely long stripe geometry by using a tight-binding model is consistent with the topological characterization based upon the isospin Chern number as well. In general, the isospin Chern number describes the topological order of the bulk electron states, which is resilient to small deformations of the system Hamiltonian, including symmetry-breaking perturbations. The isospin Chern number

can only be changed through closing either the energy gap or the isospin spectrum gap. However, it is noteworthy that while the existence of the edge states in thin films of the 3D topological insulator has its origin in the bulk topological order, the gapless nature of the edge modes is due to time-reversal symmetry.

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- ¹C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 226801 (2005).
- ²B. A. Bernevig and S. C. Zhang, *Phys. Rev. Lett.* **96**, 106802 (2006).
- ³F. D. M. Haldane, *Phys. Rev. Lett.* **61**, 2015 (1988).
- ⁴L. Sheng, D. N. Sheng, C. S. Ting, and F. D. M. Haldane, *Phys. Rev. Lett.* **95**, 136602 (2005).
- ⁵B. A. Bernevig, T. L. Hughes, and S. C. Zhang, *Science* **314**, 1757 (2006).
- ⁶M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, *Science* **318**, 766 (2007).
- ⁷C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005).
- ⁸D. N. Sheng, Z. Y. Weng, L. Sheng, and F. D. M. Haldane, *Phys. Rev. Lett.* **97**, 036808 (2006).
- ⁹L. Fu and C. L. Kane, *Phys. Rev. B* **76**, 045302 (2007); L. Fu, C. L. Kane, and E. J. Mele, *Phys. Rev. Lett.* **98**, 106803 (2007).
- ¹⁰J. E. Moore and L. Balents, *Phys. Rev. B* **75**, 121306(R) (2007).
- ¹¹D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Nature (London)* **452**, 970 (2008); D. Hsieh, Y. Xia, L. Wray, D. Qian, A. Pal, J. H. Dil, J. Osterwalder, F. Meier, G. Bihlmayer, C. L. Kane, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Science* **323**, 919 (2009).
- ¹²H. Zhang, C. Liu, X. Qi, X. Dai, Z. Fang, and S. Zhang, *Nat. Phys.* **5**, 438 (2009).
- ¹³Y. Xia, L. Wray, D. Qian, D. Hsieh, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Nat. Phys.* **5**, 398 (2009).
- ¹⁴Y. L. Chen, J. G. Analytis, J.-H. Chu, Z. K. Liu, S.-K. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, S. C. Zhang, I. R. Fisher, Z. Hussain, and Z.-X. Shen, *Science* **325**, 178 (2009).
- ¹⁵P. Roushan, J. Seo, C. V. Parker, Y. S. Hor, D. Hsieh, D. Qian, A. Richardella, M. Z. Hasan, R. J. Cava, and A. Yazdani, *Nature (London)* **460**, 1106 (2009).
- ¹⁶T. Zhang, P. Cheng, X. Chen, J.-F. Jia, X. Ma, K. He, L. Wang, H. Zhang, X. Dai, Z. Fang, X. Xie, and Q.-K. Xue, *Phys. Rev. Lett.* **103**, 266803 (2009).
- ¹⁷J. Linder, T. Yokoyama, and A. Sudbø, *Phys. Rev. B* **80**, 205401 (2009).
- ¹⁸W.-Y. Shan, H.-Z. Lu, and S.-Q. Shen, *New J. Phys.* **12**, 043048 (2010); H.-Z. Lu, W.-Y. Shan, W. Yao, Q. Niu, and S.-Q. Shen, *Phys. Rev. B* **81**, 115407 (2010).
- ¹⁹D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, *Phys. Rev. Lett.* **49**, 405 (1982); Q. Niu, D. J. Thouless, and Y. S. Wu, *Phys. Rev. B* **31**, 3372 (1985); M. Kohmoto, *Ann. Phys. (N.Y.)* **160**, 343 (1985); D. N. Sheng, L. Balents, and Z. Wang, *Phys. Rev. Lett.* **91**, 116802 (2003).
- ²⁰E. Prodan, *Phys. Rev. B* **80**, 125327 (2009).
- ²¹J. Bellissard, A. van Elst, and H. Schulz-Baldes, *J. Math. Phys.* **35**, 5373 (1994).
- ²²T. Fukui and Y. Hatsugai, *Phys. Rev. B* **75**, 121403(R) (2007); *J. Phys. Soc. Jpn.* **76**, 053702 (2007).
- ²³A. M. Essin and J. E. Moore, *Phys. Rev. B* **76**, 165307 (2007).
- ²⁴F. D. M. Haldane, *Phys. Rev. Lett.* **93**, 206602 (2004).