Dispersion of Fermi arcs in Weyl semimetals and their evolutions to Dirac cones

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We study dispersions of Fermi arcs in the Weyl semimetal phase by constructing an effective model. We calculate how the surface Fermi-arc dispersions for the top and bottom surfaces merge into the bulk Dirac cones in the Weyl semimetal at both ends of the arcs, and show that they have opposite velocities. This result is common to general Weyl semimetals, and is also confirmed by a calculation using a tight-binding model. Furthermore, by changing a parameter in the system while preserving time-reversal symmetry, we show that two Fermi arcs evolve into a surface Dirac cone when the system transits from the Weyl semimetal to the topological insulator phase. We also demonstrate that choices of surface terminations affect the pairing of Weyl nodes, from which the Fermi arcs are formed.

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I. INTRODUCTION

Topological classification of phases has been one of the fruitful ways to explore new quantum phases in condensed materials. A topological insulator (TI) is one of the topological phases in condensed materials with time-reversal (TR) symmetry [1,2]. As a manifestation of topological properties of three-dimensional TIs, their band structure is gapped in the bulk, but is gapless in the surface. The surface states are determined by topological invariants calculated from the bulk states. The topological invariants are Z_2 topological numbers defined in TR invariant systems, and the resulting gapless surface states are protected topologically.

On the other hand, more recent works have revealed another kind of topological phases, not in insulators but in semimetals: for example, Weyl semimetals (WSMs). In WSMs, the conduction and valence bands form nondegenerate Dirac cones. They touch at isolated points in k space, called Weyl nodes. Remarkably, the Weyl nodes are stable topologically, because they are associated with a topological number called a monopole charge in k space, associated with the Berry curvature in kspace. The topological WSM phases are realized in 3D systems where TR or inversion (I) symmetry is broken. As candidates of the WSMs with broken TR symmetry, pyrochlore iridates [3,4], multilayer structures consisting of TI with ferromagnetic order and normal insulator (NI) [5], and $HgCr_2Se_4$ [6] are proposed. The multilayer structure of TI and NI with an external electric field is also suggested as a candidate material for the WSM where I symmetry is broken [7]. While the WSMs have not been found experimentally yet, materials with 3D doubly-degenerate Dirac cones were recently discovered, which are called Dirac semimetals [8–11]. Because of the degeneracy, the gapless points of the Dirac semimetals are not protected topologically, unlike those of WSMs.

The number of Weyl nodes in 3D k space is necessarily even. It is because the Weyl nodes are either a monopole or an antimonopole in k space [12–14], and the sum of the monopole charge inside the Brillouin zone should vanish. Moreover, these Weyl nodes are robust topologically as long as translational symmetry is preserved.

Another remarkable topological property of WSMs is the existence of topologically protected surface states [3]. The

surface states form arcs in k space, which are called Fermi arcs, connecting between the Weyl nodes projected to the surface Brillouin zone. The appearance of Fermi arcs is explained in terms of a topological number when the Fermi energy is exactly on the Weyl nodes. As a result, the Fermi arc connects two Weyl nodes, one being a monopole and the other an antimonopole for the Berry curvature. On the other hand, the dispersion of the Weyl nodes is not well studied when the Fermi energy is away from the Weyl nodes. It is easily seen that the sign of the velocity of the Fermi-arc state is determined from the topological number, i.e., the monopole charge of the Weyl nodes, Moreover, as we find in this paper, the Fermi-arc dispersion has a unique form, which is useful to experimentally establish the WSM phase. In this paper, we discuss surface state dispersion and bulk bands by constructing a simple effective model for the WSM phase. The results from the effective model are confirmed by numerical calculations using a lattice model, which is the Fu-Kane-Mele model with an additional staggered on-site potential.

In the present paper, we discuss dispersion of surface states of the WSM phase, and their evolutions at phase transitions from the WSM phase to other bulk insulating phases such as TI phases. In particular, we focus on systems without I symmetry where WSM and TI phases are realizable. Firstly, from the effective model, we show surface Fermi arcs and their dispersions on the top surface and on the bottom surface. The top- and bottom-surface states have opposite velocities, and are tangential to bulk Dirac cones. Next, by using a lattice model realizing TI and WSM phases, we study changes of the surface states. As a result, we find that a pair of Fermi arcs evolve into a surface Dirac cone when the system moves from the WSM to the TI phase. Furthermore, the pairing of the Weyl nodes to form the Fermi arc depends on the surface termination. We also discuss how these results are applied to general WSMs.

II. WEYL SEMIMETAL PHASE CHARACTERIZED BY THE BERRY CURVATURE

To characterize WSMs, the Berry curvature in k space is important. As we explain below, the Weyl nodes are topological objects, corresponding to monopoles or antimonopoles for the

Berry curvature. This gives a strong restriction on behaviors of Weyl nodes. The Berry curvature in *k*-space is introduced as follows [12–14]. Let $\psi_{\alpha}(k)$ be the Bloch wave function and we write $\psi_{\alpha}(k) = u_{\alpha}(k)e^{ik \cdot r}$, and $u_{\alpha}(k)$ is called a periodic part of the Bloch wave function. For the α th band, the Berry connection (gauge field) $A_{\alpha}(k)$ and the corresponding Berry curvature (field strength) $B_{\alpha}(k)$ are defined as

$$A_{\alpha}(\boldsymbol{k}) = i \langle u_{\alpha}(\boldsymbol{k}) | \nabla_{\boldsymbol{k}} | u_{\alpha}(\boldsymbol{k}) \rangle, \qquad (1)$$

$$\boldsymbol{B}_{\alpha}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{A}_{\alpha}(\boldsymbol{k}), \tag{2}$$

and the corresponding monopole density is defined as

$$\rho_{\alpha}(\boldsymbol{k}) = \frac{1}{2\pi} \nabla_{\boldsymbol{k}} \cdot \boldsymbol{B}_{\alpha}(\boldsymbol{k}).$$
(3)

The properties of the monopole density are well studied [12–14]. Therefore we briefly outline its properties here. When the α th band is not degenerate with other bands at some k, the monopole density $\rho_{\alpha}(\mathbf{k})$ vanishes identically, because $u_{\alpha}(\mathbf{k})$ is analytic in the neighborhood of k. Only at the k-points where the α th band touches with another band, the monopole density can be nonzero, having a δ -function singularity. It is shown from an argument on a gauge degree of freedom that the coefficient of δ -function is always an integer, and the monopole density has the form $\rho(\mathbf{k}) = \sum_{l} q_l \delta(\mathbf{k} - \mathbf{k}_l)$, where q_l is an integer. We call the integer q_l a monopole charge. In the simplest case of $q_l = \pm 1$, it is called a monopole $(q_l = 1)$ and an antimonopole $(q_l = -1)$. The Weyl nodes are either a monopole or an antimonopole, as one can see easily from an example Hamiltonian $H = \mathbf{k} \cdot \boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. Because the monopole charge is quantized, the monopole charge cannot change under a continuous change of the Hamiltonian. They can only change at pair creation or pair annhilation of a monopole-antimonopole pair.

TR and I symmetries respectively give a restriction to these Berry curvature and monople density. The TR symmetry leads to

$$\boldsymbol{B}_{\alpha}(\boldsymbol{k}) = -\boldsymbol{B}_{\alpha_{R}}(-\boldsymbol{k}), \quad \rho_{\alpha}(\boldsymbol{k}) = \rho_{\alpha_{R}}(-\boldsymbol{k}), \quad (4)$$

where α_R is the band index obtained by time-reversal from α th band. Hence in TR-symmetric systems, monopoles are distributed symmetrically with respect to the origin k = 0. On the other hand, the I symmetry leads to

$$\boldsymbol{B}_{\alpha}(\boldsymbol{k}) = \boldsymbol{B}_{\alpha_{I}}(-\boldsymbol{k}), \quad \rho_{\alpha}(\boldsymbol{k}) = -\rho_{\alpha_{I}}(-\boldsymbol{k}), \quad (5)$$

where α_I is the band index obtained by inversion from α th band. Hence in I-symmetric systems, monopoles are distributed antisymmetrically with respect to the origin $\mathbf{k} = 0$. Furthermore, in systems with both TR and I symmetries, all states are doubly degenerate by Kramers theorem, and therefore a Dirac cone without degeneracy is impossible. Therefore the WSM requires either breaking of TR symmetry or that of I symmetry, as has been proposed [5,15]. Such systems with broken TR or I symmetries can be realized as multilayers of TIs and NIs [5,7,15].

III. EFFECTIVE MODEL FOR THE NI-SW-TI PHASE TRANSITION

To describe a WSM and its evolution under a change of Hamiltonian parameters, we construct a minimal model including only a single valence band and a single conduction band. Therefore we consider a minimal model described by a 2×2 matrix $H(\mathbf{k},m)$, where *m* is introduced as a control parameter for NI-WSM-TI phase transition. The 2×2 Hamiltonian $H(\mathbf{k},m)$ is expanded as

$$H(\boldsymbol{k},m) = a_0(\boldsymbol{k},m) + \sum_{i=1}^3 a_i(\boldsymbol{k},m)\sigma_i, \qquad (6)$$

where σ_i (*i* = 1,2,3) are the Pauli matrices representing conduction and valence bands. The gap between the two eigenvalues closes when the three conditions

$$a_i(\mathbf{k},m) = 0 \ (i = 1,2,3)$$
 (7)

are satisfied. If Eq. (7) has solutions for k at a given value of m, the bands generally form a Dirac cone without degeneracy at these k points, if $\frac{\partial(a_1,a_2,a_3)}{\partial(k_x,k_y,k_z)} \neq 0$. Therefore it is generally a WSM and the respective Weyl nodes are monopoles or antimonopoles, depending on the monopole charge equal to $\operatorname{sgn} \frac{\partial(a_1,a_2,a_3)}{\partial(k_x,k_y,k_z)} = \pm 1$.

Let us then change the parameter *m*. In order to open a gap in the system, all the monopoles and antimonopoles should disappear via monopole-antimonopole pair annihilation. Conversely, if we begin with a system with a bulk gap at some parameter *m*, and if a change of *m* induces appearance of Weyl nodes, then it should involve monopole-antimonopole pair creation. One of the purposes of the present paper is to create a simple effective model describing the WSM phase close to monopole-antimonopole pair creation or annihilation, i.e., near the phase transition between the WSM phase and a bulk insulating phase. Let $m = m_0$ be the value of *m* where this monopole-antimonopole pair creation occurs. A part of the formalism here follows the previous paper by one of the authors [16].

Suppose we change the value of *m* through the phase transition between the WSM phase and a phase with a bulk gap. It is accompanied by a pair creation or annihilation, and let m_0 denote the value of *m* where the phase transition occurs. Then on one side of *m*, e.g., $m < m_0$, the system is a WSM with an monopole and antimonopole, while on the other side of *m*, e.g., $m > m_0$, the system is an insulator in the bulk, which can be a NI or a TI. At $m = m_0$, the gap closes at some point where the pair creation occurs, and let $\mathbf{k} = \mathbf{k}_0$ denote the point; namely, it satisfies $\mathbf{a}(\mathbf{k}_0, m_0) = 0$. We expand the coefficients of Eq. (6) to the linear order around \mathbf{k}_0 and m_0 :

$$\boldsymbol{a}(\boldsymbol{k},m) = \boldsymbol{M}\Delta\boldsymbol{k} + \Delta m\boldsymbol{N},\tag{8}$$

where $\Delta k_j = k_j - k_{0j}$, $\Delta m = m - m_0$, and $M_{ij} = \frac{\partial a_i}{\partial k_j}|_0$ and $N_i = \frac{\partial a_i}{\partial m}|_0$ are the values of derivatives at $m = m_0$ and $k = k_0$. It gives a generic Hamiltonian describing a pair creation of monopoles at $m = m_0$, shown in Ref. [16]. From this Hamiltonian we can calculate the motion of the Weyl nodes close to the pair creation (i.e., the phase transition between the WSM and the bulk insulating phase), and band dispersions [16].

It is also noted in Ref. [16] that pair creations occur in pairs at $k = k_0$ and $k = -k_0$ simultaneously, imposed by Eq. (4). Thus there are at least two monopoles and two antimonopoles in the WSM with TR symmetry (but without I symmetry). If one varies *m* further and the system becomes a bulk insulating phase again, there should be pair annihilations to make all the monopoles and antimonopoles disappear. If pair annihilations occur by exchanging partners from the pair creations, some of the four Z_2 topological numbers of 3D TIs should be different between the initial bulk-insulating phase and the final bulkinsulating phase.

Our goal here is to calculate an evolution of surface states through this change of the WSM phase. To this goal, the generic Hamiltonian described above is not convenient because it contains many parameters. Therefore, instead of using the above generic Hamiltonian, we use a simplified Hamiltonian. This is obtained from the above Hamiltonian after some gauge transformation, scale transformation, and a few simplifying assumptions. The details of this derivation is in Appendix. The resulting effective model is described by a Hamiltonian

$$H = \gamma \left(k_x^2 - m\right)\sigma_x + v(k_y\sigma_y + k_z\sigma_z),\tag{9}$$

where v and γ are nonzero constants, and we choose them to be positive for simplicity. In deriving this model, among Weyl nodes in the WSM, we focused on one monopole and one antimonopole, which are assumed to be close to each other. We then shifted the origin of the wave vector to simplify the Hamiltonian and retained terms that are of the lowest order in k. Therefore this Hamiltonian generally applies to any WSMs, i.e., those with I symmetry breaking or those with TR symmetry breaking, as long as a monopole and an antimonopole are close to each other. We note that the origin of the wave vector in this Hamiltonian does not correspond to k = 0 in the original Bloch wave vector due to the shifting. Therefore symmetry properties of the Hamiltonian H, such as I or TR symmetries, cannot be discussed in Eq. (9). Its bulk dispersion is given by

$$E = \pm \sqrt{\gamma^2 (k_x^2 - m)^2 + v^2 k_y^2 + v^2 k_z^2}.$$
 (10)

The Fermi energy is assumed to be at E = 0. When m < 0 it describes a phase with a bulk gap $2\gamma |m|$, either the TI or the NI phase. On the other hand, when m > 0, the bulk gap closes at two points W_{\pm} : $\mathbf{k} = (\pm \sqrt{m}, 0, 0)$. Around these points, the dispersions are linear in three directions, and therefore they describe the WSM phase. These two Weyl nodes W_{+} and W_{-} are a monopole and an antimonopole for the lower band, respectively. At m = 0, there occurs a monopole-antimonopole pair creation. Hence this effective Hamiltonian describes one pair creation/annihilation of a monopole and an antimonopole when the phase transition occurs.

Let us consider a surface of the WSM phase with $m = m_0(> 0)$. Following the standard technique, we describe the surface by a space-dependent value of m. Namely, we regard m to change its sign at the surface. We set m to have a negative value in the vacuum side, and m converges to m_0 (>0) in the WSM side. The surface is assumed to be along the xy plane

for simplicity. Therefore we set

$$m(z) = m_0 \quad : z \to -\infty, m(z) < 0 \quad : z \to +\infty,$$
(11)

for the surface normal to be $+\hat{z}$, which we call a top surface, and

$$m(z) < 0 \qquad : z \to -\infty, m(z) = m_0 \qquad : z \to +\infty,$$
(12)

for the surface normal to be $-\hat{z}$, which we call a bottom surface. They correspond to the top and bottom surfaces of a slab with sufficiently large thickness.

Here we calculate band dispersions for the top surface and for the bottom surface. By unitary transformation with $U = \frac{1}{\sqrt{2}}(1 - i\sigma_x)$, the Hamiltonian is transformed to

$$H' \equiv U^{-1}HU = \gamma \left(k_x^2 - m\right)\sigma_x - iv\frac{\partial}{\partial z}k_z\sigma_y - vk_y\sigma_z$$
$$= \begin{pmatrix} -vk_y & \gamma \left(k_x^2 - m\right) - v\frac{\partial}{\partial z}\\ \gamma \left(k_x^2 - m\right) + v\frac{\partial}{\partial z} & vk_y \end{pmatrix}.$$
 (13)

Because we focus on the surface within the xy plane, we have replaced k_z with $-i\frac{\partial}{\partial z}$, while k_x and k_y are the Bloch wave numbers. It is now straightforward to write down the eigenstates bound to the surfaces. The bound state on the top surface is given by

$$\psi_{\mathrm{T}} = \begin{pmatrix} 1\\ 0 \end{pmatrix} e^{-(\gamma/\nu)\int^{z} (k_{x}^{2} - m(z))dz}, \quad E = -\nu k_{y} \qquad (14)$$

and the bound state on the bottom surface is given by

$$\psi_{\mathrm{B}} = \begin{pmatrix} 0\\1 \end{pmatrix} e^{(\gamma/\nu)\int^{z} (k_{x}^{2} - m(z))dz}, \quad E = \nu k_{y}.$$
(15)

They are respectively allocated as top- and bottom-surface states, because otherwise the wave function diverges at some region and is not normalizable. We also note that both of these surface states exist only when

$$-\sqrt{m_0} < k_x < \sqrt{m_0}. \tag{16}$$

At E = 0, the surface states are degenerate, and are located at $k_y = 0$, $-\sqrt{m_0} < k_x < \sqrt{m_0}$, which is a line connecting the 2D projection of the Weyl points W_{\pm} : $\mathbf{k} = (\pm\sqrt{m_0}, 0, 0)$. Thus these surface states are Fermi arcs. We note that the top-surface Fermi-arc states have a velocity $\mathbf{v} = \frac{\partial E}{\partial \mathbf{k}} = (0, -v)$ and those of the bottom-surface have a velocity $\mathbf{v} = \frac{\partial E}{\partial \mathbf{k}} = (0, v)$. Their signs are consistent with the fact that W_{\pm} are a monopole and an antimonopole, respectively. The velocity signs follow from the fact that on the slice of the 3D BZ at $k_x = \text{const.}$, the lower band has a Chern number 0 for $\sqrt{m_0} < |k_x|$ and -1 for $-\sqrt{m_0} < k_x < \sqrt{m_0}$ due to the antimonopole at W_{1-} .

We show how these surface states disperse if the Fermi energy is away from the Weyl point. To see how the bulk bands and surface bands are related, we project the bulk dispersion, Eq. (10), onto the surface. The resulting bulk bands are in regions

$$E > \sqrt{\gamma^2 (k_x^2 - m_0)^2 + v^2 k_y^2},$$
 (17)

$$E < -\sqrt{\gamma^2 (k_x^2 - m_0)^2 + v^2 k_y^2},$$
 (18)

which describe the conduction and the valence bands, respectively. These two bands touch each other at the projections of the two Weyl nodes W_{\pm} : $k_x = \pm \sqrt{m_0}$, $k_y = 0$. Around these Weyl nodes the dispersion is linear. This projected bulk band structure is shown in Fig. 1(a), forming two Dirac cones around the Weyl nodes W_{\pm} . The surface states are tangential to these cones, as shown in Fig. 1(b). A similar surface-state dispersion was proposed in Ref. [3] without calculations, and our calculation on the effective model confirms this dispersion of surface states. We also note that similar results have been independently obtained in Ref. [17] for a toy model. Our results are based on generic considerations (see Appendix) from an effective model (9), and are applicable to general WSM.

To see the relationship between the projection of the bulk bands and the surface states, we show the Fermi surface at a constant energy E. The bulk-band projection changes its topology at $E = \pm \gamma m_0$. When $-\gamma m_0 < E < \gamma m_0$, the bulk-band projection forms two distinct pockets as shown in Fig. 1(c), and the Fermi arcs are bridged between these two pockets. When $|E| > \gamma m_0$, it forms one pocket with a dumbbell-like structure [Fig. 1(d)]. In either case, it is remarkable that the Fermi arc merges to the bulk-band projection at the two ends, and at both ends they are tangential to the bulk-band projection.

We note that the obtained dispersions of surface and bulk states are generic as long as the monopole and the antimonopole are close to each other. It is because the Hamiltonian is derived from generic considerations by expanding the Hamiltonian in terms of the wave vector close to the monopole-antimonopole pair creation point, with scale transformation. Hence we expect that this dispersion holds for general WSMs with a pair of Weyl nodes that are close to each other.



FIG. 1. (Color online) Bulk and surface states of the model for the WSM. The parameters are set as $v = \gamma = m_0 = 1$. (a) shows the bulk states, and (b) shows the surface Fermi arcs and the bulk states. (c) and (d) The Fermi surface for the Fermi energy at (c) E = 0.5 and at (d) E = 1.5.

IV. NUMERICAL CALCULATION OF SURFACE STATES OF WEYL SEMIMETALS IN A LATTICE MODEL

A. Model

In this section, we numerically calculate surface states in a WSM phase and compare the results to the discussions in Sec. III. For this purpose, we begin with the Fu-Kane-Mele (FKM) tight-binding model [18], which is known to show various 3D TI phases. It does not show the WSM phase as it is, because it does not break I symmetry. By adding a staggered on-site potential to the model to break I symmetry, it does show the WSM phase as shown in Ref. [16]. It was later used also in Ref. [19] to calculate surface Fermi arcs in some parameter range.

Hence we use the FKM model with a staggered on-site potential added. Our model is a 3D tight-binding model on a diamond lattice, described by the following Hamiltonian:

0.

$$H = \sum_{\langle i,j \rangle} t_{ij} c_i^{\dagger} c_j + i \frac{8\lambda_{so}}{a^2} \sum_{\langle \langle i,j \rangle \rangle} c_i^{\dagger} s \cdot (\boldsymbol{d}_{ij}^1 \times \boldsymbol{d}_{ij}^2) c_j + \lambda_v \sum_i \xi_i c_i^{\dagger} c_i, \qquad (19)$$

where *s* are Pauli matrices and *a* is the lattice constant for the cubic unit cell. The first term is the nearest-neighbor hopping with hopping amplitude t_{ij} . The second term represents the spin-orbit interaction for next-nearest-neighbor hopping with a spin-orbit coupling parameter λ_{so} . d_{ij}^1 and d_{ij}^2 are the nearest-neighbor vectors connecting second-neighbor sites *i* and *j*. The third term represents the staggered on-site energy $\pm \lambda_v$, where λ_v is a constant and $\xi_i = \pm 1$ depends on the sublattices, i.e., $\xi = +1$ for the A sublattice and $\xi = -1$ for B sublattice for the diamond lattice.

The model without the third term is the FKM model, and is TR and I symmetric [18]. Provided the nearest-neighbor hoppings t_{ij} are identical, the FKM model has gapless band structure with the bulk gap closed at the three X points, showing that it is a Dirac semimetal. There are four directions of the nearest-neighbor bonds, and when the hopping integrals for four nearest-neighbor bonds t_{α} ($\alpha = 1,2,3,4$) become different, the model shows various phases of either strong topological insulator (STI) or weak topological insulator (WTI) phases. The hopping integrals along the bond in the 111, 111, 111, and 111 directions are denoted as t_1, t_2, t_3 , and t_4 , respectively.

To realize the WSM phase with TR symmetry, the system needs to be I-asymmetric. In Ref. [16], it is shown that with the λ_v term breaking the I-symmetry, this model shows the WSM phase. The Hamiltonian matrix is

$$\mathcal{H}(\boldsymbol{k}) = \begin{pmatrix} \lambda_{\nu} \mathbf{1} + \sum_{i=1}^{3} F_{i} s_{i} & f \mathbf{1} \\ f^{*} \mathbf{1} & -\lambda_{\nu} \mathbf{1} - \sum_{i=1}^{3} F_{i} s_{i} \end{pmatrix}, \quad (20)$$

where

$$f = t_1 + t_2 e^{ik \cdot a_2} + t_3 e^{ik \cdot a_3} + t_4 e^{ik \cdot a_1},$$
(21)

$$F_x = -4\lambda_{\rm so}\sin\frac{a}{2}k_x\left(\cos\frac{a}{2}k_y - \cos\frac{a}{2}k_z\right),\qquad(22)$$

and F_y and F_z are given by cyclic permutation of the subscripts x, y, and z in F_x . The primitive vectors of the fcc lattice are defined as $a_1 = \frac{a}{2}(1,1,0)$, $a_2 = \frac{a}{2}(0,1,1)$, $a_3 = \frac{a}{2}(1,0,1)$. The energy eigenvalues are

$$E(\mathbf{k}) = \pm \sqrt{(\lambda_v \pm |\mathbf{F}|)^2 + |f|^2},$$
(23)

where $F = (F_x, F_y, F_z)$. Therefore the spectrum is gapless when

$$\operatorname{Re} f = \operatorname{Im} f = 0, \ \lambda_v = \pm |\boldsymbol{F}|.$$
(24)

In some parameter region, the three equations (24) for three parameters k_x , k_y , and k_z have solutions, showing the locations of the Weyl nodes. The bulk gap is then closed and the WSM phase appears there.

B. Numerical calculation of surface states

In Ref. [16], phase diagrams of this model are studied and this model is shown to exhibit the STI, WTI, and WSM phases by changing parameters. As an example, we assume $t_1 = t + \delta t_1$, $t_2 = t + \delta t_2$, $t_3 = t_4 = t$, and $\delta t_- = \delta t_1 - \delta t_2$ is fixed to be positive while $\delta t_+ = \delta t_1 + \delta t_2$ is varied. For the case with I symmetry, i.e., $\lambda_v = 0$, a band inversion at $X^x = \frac{2\pi}{a}(1,0,0)$ occurs at $\delta t_+ = 0$, accompanied by a phase transition between the STI phase with the Z_2 topological number 1;(111) ($\delta t_+ > 0$) and the WTI phase with the Z_2 topological number 0;(111) ($\delta t_+ < 0$) [18]. As a result, when the system is in the STI phase, a surface Dirac cone arises at the point $X^x = \frac{2\pi}{a}(1,0,0)$ projected onto the surface Brillouin zone, while in the WTI phases there is no surface Dirac cone at this point.

If one introduces an on-site staggered potential λ_v , the I symmetry is broken while the TR symmetry is preserved. Then the WSM phase intervenes between the STI and the WTI phases, as shown in Fig. 2(a). In the WSM phase, there are four Weyl nodes around the X^x point, as found in Ref. [16]. These four Weyl nodes move as the parameter $\delta t_+ = \delta t_1 + \delta t_2$ changes. Among these four Weyl nodes, two are monopoles and the other two are antimonopoles, which distribute symmetrically with respect to the X^x point. On the surface, two Fermi arcs will arise, connecting monopole-antimonopole pairs. For calculations, we fix $\delta t_- = \delta t_1 - \delta t_2 = 0.1t$ and $\lambda_{so} = 0.1t$.

To see surface states, we numerically diagonalize Eq. (19) in a slab geometry with (111) surfaces. To show the surface states, we take the *z* axis to be the surface normal along [111], the *x* axis along the surface in the a_3 - a_1 direction and the *y* axis to be perpendicular to the *x* and *z* axes. The top surface of the slab is composed of lattice sites in the sublattice A and the bottom surface is composed of lattice sites in the sublattice B. Because the point X^x is projected to the point $M_2 = \frac{2\pi}{b}(0, 1/\sqrt{3})$ in the hexagonal surface Brillouin zone, the Dirac cones and the Fermi arcs appear around the point M_2 . Here, $b = a/\sqrt{2}$ is the length of the primitive vectors of the slab.

Figures 2(b)–2(d) shows Fermi surfaces of a slab at E = 0for various values of δt_+ , with $\delta t_- = 0.1t$ and $\lambda_{so} = 0.1t$. For (b) $\delta t_+ = 0$ and (c) $\delta t_+ = 0.03$, the system is in the WSM phase, and Fermi arcs appear around point M_2 , corresponding to point X^x . The ends of arcs are the Weyl nodes projected into the surface Brillouin zone. Among the four Weyl points,



FIG. 2. (Color online) (a) Phase diagram in the $\delta t_+ -\lambda_v$ plane, with $\delta t_- = 0.1t$ and $\lambda_{so} = 0.1t$, where $\delta t_{\pm} = \delta t_1 \pm \delta t_2$. The axes are in the unit of t. When $\lambda_v = 0$, the system is I-symmetric, and no WSM phase appears. (b)–(d) Surface Fermi surface at E = 0 around the point M_2 near the Fermi level with $\lambda_v = 0.2t$ and the following values for δt_+ : (b) $\delta t_+ = 0$ (WSM), (c) $\delta t_+ = 0.03t$ (WSM), and (d) $\delta t_+ = 0.05t$ (STI). The axes are in the unit of $2\pi/b$. (b) and (c) show Fermi arcs in the WSM phase, and (d) shows a surface Dirac cone in the STI phase. We note that the end points of the surface Fermi arcs in the WSM phase are the gapless points of the bulk bands.

let W_{1+} and W_{2+} denote the monopoles, and let W_{1-} and W_{2-} denote the antimonopoles, which are shown in Figs. 2(b) and 2(c). As δt_+ is changed, the Weyl nodes move around this M_2 points, and concomitantly the Fermi arcs grow as seen in Figs. 2(b) and 2(c). As δt_+ is increased further, the system eventually enters the STI phase. At the WSM-STI phase transition, the Weyl nodes annihilate pairwise for (W_{1-}, W_{2+}) and (W_{1+}, W_{2-}), and there is no Weyl node in the STI phase, with a nonzero bulk gap. Correspondingly, as we see in Fig. 2(d), the two Fermi arcs in the WSM phase are merged into a surface Dirac cone in the STI phase.

We discuss a relationship between the present work and the paper by Ojanen [19]. In the present work we fix the spin-orbit coupling λ_{so} to be a constant and change the anisotropy of the nearest-neighbor hoppings. It enables us the phase transitions from the WSM phase to either the STI or the WTI phases. On the other hand, in Ojanen's paper [19], the spin-orbit parameter λ_{so} is changed across zero, to see the NI-WSM phase transitions. In approaching the WSM-NI phase transition, the Fermi arcs are gradually shortened and eventually vanish.

So far, we have discussed the surface states on E = 0, where the states on the top surface and those on the bottom surface are degenerate. The top-surface states and bottom-surface states are expected to have different dispersions, as Fig. 1(b) shows. Figure 3 shows the results for the dispersion of the Fermi arcs on the top- and bottom-surface states in the present model. We note that the top- and bottom-surface states between a pair of Weyl nodes have opposite velocities, and the signs of the velocities are consistent with the monopole charges of $W_{i\pm}$ (i = 1,2). To see this, let us focus on the surface Fermi



FIG. 3. (Color online) Side views of the Fermi arcs around point $M_2 = \frac{2\pi}{b}(0, 1/\sqrt{3})$ with $\lambda_v = 0.2t$, $\delta t_+ = 0$ (WSM phase) for (a) the top surface and (b) the bottom surface. The k_x and k_y axes are in the unit of $2\pi/b$. The red (blue) points are the gapless points, which have positive (negative) monopole charges for the Berry curvature.

arc between W_{1+} and W_{1-} as an example, and ignore the other Fermi arc. Let us take a 2D slice of the 3D Brillouin zone, which includes the surface normal ([111] direction). If the slice does not intersect the line between $W_{1\pm}$, the Chern number is zero within this 2D slice, while it is one when the slice intersects the line between $W_{1\pm}$ because of the presence of the monopole at W_{1+} . This means that within this slice there should be a clockwise topological edge mode, which appears as a surface mode with negative velocity $v_x < 0$ on the top surface and that with positive velocity $v_x > 0$ on the bottom surface. As is consistent with the result of the effective model [Fig. 1(b)], each of these surface Fermi arcs is bridged between two Dirac cones around the Weyl nodes. As δt_{+} is increased and the system undergoes the phase transition from the WSM phase into the STI phase, the two Fermi arcs merge into a single Dirac cone on the top surface, and the same occurs on the bottom surface. As a result there arises a topsurface Dirac cone and a bottom-surface Dirac cone, which are nondegenerate as shown schematically in Fig. 4(a). This splitting of the Dirac cones are natural, because of the breaking of the I-asymmetry due to the staggered on-site energy λ_v . In the present case, the topmost layer in the top (bottom) surface is A sublattice (B sublattice), and therefore the top-surface (bottom-surface) states have a larger (smaller) energy due to the staggered on-site energy λ_v .



FIG. 4. (Color online) Schematic drawing of the surface energy bands around a TRIM. The red (green) cone is the top (bottom) surface states. (a) In the STI phase, the two Dirac cones on the top and bottom surfaces are split in energy when the I symmetry is broken. (b) In the WSM phase, there are a pair of Fermi arcs on each surface. These Fermi arcs will evolve into a Dirac cone shown in (a) in the STI phase.

The surface states in the whole BZ for $\delta t_+ = 0$ (WSM) and $\delta t_+ = 0.05t$ (STI) when $\lambda_v = 0.2t$ are shown in Figs. 5(a1) and 5(b1). In addition to the surface states around M_2 , there are Dirac cones around M_1 and M_3 . Nevertheless, they are intact at the WTI-WSM-STI phase transition, because this phase transition is related with a band inversion at X_x , which is projected onto M_2 point.

C. WSM-TI phase transition and evolution of the Fermi-arc surface states

Based on the calculation results on the model (19), here we discuss general features of the evolution of the Fermi-arc surface states in the WSM phase when some parameter is changed. In the WSM phase there are an even number of Weyl nodes. In the I-asymmetric phases with TR symmetry, the minimal number is four, i.e., two monopoles and two antimonopoles, as follows from Eq. (4). In this case of two monopoles and antimonopoles, symmetrically distributed around a TRIM k_{Γ} , the Fermi arcs are formed between monopole-antimonopole pairs, as exemplified in Fig. 2. Suppose then we change some parameter in the system. Due to topological nature



FIG. 5. (Color online) The surface Fermi surfaces at E = 0 in the whole BZ when $\lambda_v = 0.2t$. The values of δt_+ is $\delta t_+ = 0$ (WSM) for (a1) and (a2), and $\delta t_+ = 0.05t$ (STI) for (b1) and (b2). In (a1) and (b1), the surfaces are terminated without dangling bonds, and in (a2) and (b2) with dangling bonds. The insets show the magnified images of the surface Fermi surface around the M_2 point.

of Weyl nodes, the monopoles and antimonopoles move in the 2D surface BZ. Eventually, they may undergo some pair annihilations, which occur symmetrically with respect to the TRIM k_{Γ} ; the bulk bands become gapped. If a pair annihilation occurs for a pair connected by a Fermi arc, the Fermi arc eventually vanishes and the surface becomes gapped. On the other hand, if the pair annihilation occurs between a monopole and an antimonopole, which are not connected to each other by the Fermi arc, the pair annihilations will make all the Fermi arcs into a single loop encircling the TRIM k_{Γ} . This loop constitutes a Dirac cone around the TRIM.

From the viewpoint of the change of the Z_2 topological number and associated surface states, the evolution of the surface states accompanying the WTI-STI topological phase transition occurs in the following way. When the I-symmetry is broken, there should generally arise a WSM phase between the WTI-STI phase transition. In the WTI-WSM phase transition, two pairs of Weyl nodes are created close to a TRIM k_{Γ} [14]. As the system enters the WSM phase, a Fermi arc is formed between the two Weyl nodes within each pair. Thus there are two Fermi arcs, which are symmetric with respect to the TRIM. As a control parameter is changed, the Fermi arcs grow as the Weyl nodes travel around the TRIM. Eventually, at the WSM-STI phase transition, the four Weyl nodes annihilate pairwise, causing a fusion of two Fermi arcs into a single Dirac cone encircling the TRIM, as shown by Fig. 4.

In Ref. [20], it is argued that when I symmetry is preserved, a Z_2 topological index defined for each surface TRIM indicates whether the focused surface TRIM is inside or outside the surface Fermi surface. It is also concluded that this index depends on the surface termination. Within this argument in Ref. [20], the surface should include the inversion center, and therefore there are two possible surface terminations for a fixed surface orientation. If we change one surface termination into the other, surface TRIM which were inside the Fermi surface will become outside the Fermi surface, and vice versa. We now try to apply this scenario to our model. However, the I symmetry is broken in our model, and the discussion in Ref. [20] is not directly applied, Nevertheless, we can expect the similar physics from continuity argument, by switching on the I-symmetry breaking. For example, in Figs. 5(a1) and 5(b1), we show the Fermi surface on the (111) surface with the surface terminated with the atoms, each of which has three bonds along $1\overline{1}\overline{1}$, $\overline{1}1\overline{1}$, and $\overline{1}\overline{1}1$. In this surface termination, the top surface is terminated by atoms in the A sublattice, and the bottom surface by atoms in the B sublattice. By adding bonds (i.e., "dangling bonds") along 111 directions to the topmost atoms, we can switch from one surface termination to the other, namely, the top and the bottom surfaces terminated by B and A sublattices, respectively. The results are plotted in Figs. 5(a2)and 5(b2), whose parameters are identical with (a1) and (b1), respectively. We can see that the physics discussed in Ref. [20] carries over to the present model as well. For example, the M_1 and M_3 points are inside the Fermi surfaces when the dangling bonds are absent [Figs. 5(a1) and 5(b1)], but when the dangling bonds are added, the Fermi surfaces around the M_1 and M_3 points disappear [Figs. 5(a2) and 5(b2)]. On the other hand, there appears a new Fermi surface around the Γ point when the dangling bonds are added. The remarkable phenomenon occurs around the M_2 point. The Fermi surface around the M_2 point in the STI phase in (b1) disappears in the plot (b2) where the dangling bonds are present. This also affects the neighboring WSM phase, as can be seen by comparing (a1) and (a2). Among the Weyl nodes in (a1) the Fermi arcs arise between W₁₊-W₁₋ and between W₂₊-W₂₋. Meanwhile in (a2), the Fermi arcs arise between W₁₊-W₂₋ and between W₂₊-W₁₋. Thus we have shown that the change of surface termination exchanges the pairs of Weyl nodes, out of which the Fermi arcs are formed.

This change of pairing of Weyl nodes by varying surface terminations occurs in generic WSMs. The Dirac cones in TIs depend on surface terminations, as shown in Ref. [20]. Because the WSM phase is next to the TI phase [14,16], the dependence on the surface termination in general WSMs (with TR symmetry) follows from that in the TIs, as we discussed in this paper. When the surface termination is varied, the pairing of the Weyl nodes will change, and the union of the pairing of the Weyl nodes before and after the change of surface termination forms a loop, which turns out to be the surface Fermi surface in the TI phase around a particular TRIM. In the present case, the pairing is $\{(W_{1+}, W_{1-}), (W_{2+}, W_{2-})\}$ or $\{(W_{1+}, W_{2-}), (W_{2+}, W_{1-})\}$, depending on the surface termination, and their union forms a loop around the M_2 point. This also implies that the pairing of the Weyl nodes for the Fermi arc is not solely determined from bulk band structure, because it depends on surface terminations.

V. CONCLUSION

In the present paper, we study dispersions of Fermi arcs in the Weyl semimetal phase. We first construct a simple effective model, describing the Weyl semimetal with two Weyl nodes close to each other. We find that the dispersions of Fermi-arc states for top- and bottom surfaces cross around the Weyl point, and they have opposite velocities. These Fermi-arc dispersions are tangential to the bulk Dirac cones around the Weyl points. These results are confirmed by a calculation using a tight-binding model with time-reversal symmetry but without inversion symmetry. In this model calculations, we see that the Fermi arcs gradually grow by changing a model parameter, and that two Fermi arcs finally merge together to form a single Dirac cone when the system transits from the Weyl semimetal to the topological insulator phase. We also find that by changing the surface termination, the pairing between the two monopoles and two antimonopoles to make Fermi arcs is switched. These results reveal an interesting interplay between the surface and the bulk electronic states in Weyl semimetals and topological insulators.

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APPENDIX: EFFECTIVE MODEL CLOSE TO MONOPOLE-ANTIMONOPOLE PAIR CREATION OR ANNIHILATION IN *k* SPACE

From the Hamiltonian (6) with (8), one can derive an effective model describing the WSM phase close to a monopoleantimonopole pair creation/annihilation. The argument closely follows that in Ref. [16]. We note that Δm is a control parameter for the Hamiltonian, and our goal is to construct a Hamiltonian where positive and negative Δm represents the WSM and the bulk insulating phases, respectively. First, we note that the determinant of the matrix M in (8) is zero, because otherwise the gapless condition (7) guarantees existence of kfor both the positive and the negative values of Δm , meaning that both the positive and negative sides of Δm are conducting in the bulk. Hence we have det M = 0, and, therefore, the matrix M has a unit eigenvector n_1 with zero eigenvalue: $M\mathbf{n}_1 = 0$. In Ref. [16], an orthonormal basis $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ is constructed out of this unit vector n_1 . While we can, in principle, proceed here as in Ref. [16], it leaves a number of free parameters in the model. In fact, we can always set $\mathbf{n}_1 = {}^t(1,0,0), \, \mathbf{n}_2 = {}^t(0,1,0), \, \mathbf{n}_3 = {}^t(0,0,1), \, \text{by a rotation of } \mathbf{k}$ coordinate axes. Then from (8) to the linear order in Δk and *m*, we have

$$\boldsymbol{a} = \Delta k_{\boldsymbol{v}} \boldsymbol{u}_2 + \Delta k_{\boldsymbol{z}} \boldsymbol{u}_3 + \Delta \boldsymbol{m} \boldsymbol{N}, \tag{A1}$$

where $u_i = Mn_i$ (i = 2,3). The gap closes when a = 0, but it cannot happen in general for $\Delta m \neq 0$ because the three vectors u_2, u_3, N are generally linearly independent. It is an artifact of

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retaining only the linear terms in Δm and Δk . Thus we have to include the next order in Δk and Δm . It turns out that the only relevant term here is the quadratic term in Δk_x [16] and therefore we additionally retain only this term, to obtain

$$\boldsymbol{a} = \Delta m \boldsymbol{N} + \Delta k_y \boldsymbol{u}_2 + \Delta k_z \boldsymbol{u}_3 + (\Delta k_x)^2 \boldsymbol{u}_{11}, \qquad (A2)$$

where γ and v are positive constants. The gap closes when this vector is zero. The solution can be written down explicitly for generic cases, but instead we here introduce a simplifying assumption:

$$\boldsymbol{u}_{11} = -N = \begin{pmatrix} \gamma \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{u}_2 = \begin{pmatrix} 0 \\ v \\ 0 \end{pmatrix}, \quad \boldsymbol{u}_3 = \begin{pmatrix} 0 \\ 0 \\ v \end{pmatrix}.$$
 (A3)

Namely, u_{11} and N are parallel, and they are orthogonal to u_2 and u_3 . Then we get

$$\boldsymbol{a} = \begin{pmatrix} \gamma [(\Delta p_1)^2 - m] \\ \upsilon \Delta p_2 \\ \upsilon \Delta p_3 \end{pmatrix}.$$
 (A4)

It is straightforward to see that the solution for this exists only when *m* is positive. This means that positive *m* represents the WSM phase while negative *m* means a bulk insulating phase. Within the WSM phase, the Weyl nodes are given by $(\Delta k_x, \Delta k_y, \Delta k_z) = (\pm \sqrt{m}, 0, 0)$. If we have not employed the simplifying assumptions Eq. (A3), there arise terms in the expressions of the Weyl nodes, which are linear in *m* [16]. Nevertheless, these terms are not the main focus of the paper, and we discard them for simplicity for illustration of surface state dispersions and evolutions.

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