Interface metallic states between a topological insulator and a ferromagnetic insulator

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We study electronic structures at an interface between a topological insulator and a ferromagnetic insulator by using a three-dimensional two-band model. In usual ferromagnetic insulators, the exchange potential is much larger than the bulk gap size in the topological insulators and electronic structures are asymmetric with respect to the Fermi level. In such situation, we show that unusual metallic states appear under the magnetic moment pointing the perpendicular direction to the junction plane, which cannot be described by the two-dimensional effective model around the Dirac point. When the magnetic moment is in the parallel direction to the plane, the number of Dirac cones becomes even integers. The conclusions obtained in analytical calculations are confirmed by numerical simulations on tight-binding lattice.

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I. INTRODUCTION

Physics of a metallic state on a surface of a three-dimensional (3D) topological insulator (TI)\textsuperscript{1–4} is undoubtedly a hot issue these days.\textsuperscript{5–7} Intrinsic phenomena originated from the topological nature of the insulating state would open a novel field of condensed matter physics. In particular, the metallic surface state shows interesting features when the TI is attached to another materials with gapped excitation spectra such as superconductors\textsuperscript{8–10} and ferromagnetic insulators.\textsuperscript{11–16}

We study electronic states at the interface between a topological insulator and a ferromagnetic insulator (FI) by using a three-dimensional two-band model. In usual ferromagnetic insulators, the exchange potential is much larger than the bulk gap size in the topological insulators and electronic structures are asymmetric with respect to the Fermi level. In such situation, we show that unusual metallic states appear under the magnetic moment pointing the perpendicular direction to the junction plane, which cannot be described by the two-dimensional effective model around the Dirac point. When the magnetic moment is in the parallel direction to the plane, the number of Dirac cones becomes even integers. The conclusions obtained in analytical calculations are confirmed by numerical simulations on tight-binding lattice.

II. EFFECTIVE THEORY AROUND THE DIRAC POINT

We firstly summarize the features of the interface state which have been discussed by using effective Hamiltonian around the Dirac point in two dimensions.\textsuperscript{1,3} The effective Hamiltonian in two dimensions is derived from the three-dimensional electric states of a TI described by

$$ H = \left( \begin{array}{cc} A \delta_0 & d(k) \cdot \hat{s} \\ d(k) \cdot \hat{s} & -A_0 \delta_0 \end{array} \right), $$

$$ A = M_0 - \sum_\alpha B_\alpha k_\alpha^2, $$

where $M_0$ and $B_\alpha$ for $\alpha = 1–3$ are band parameters. The unit matrix in spin space is denoted by $\delta_0$ and $\delta_\alpha$ for $\alpha = 1–3$ are the Pauli matrices. The spin-orbit coupling is symbolically expressed by $d(k)$, which satisfies

$$ d(-k) = -d(k). $$

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The surface state on the TI is approximately described by the effective Hamiltonian in two dimensions:

\[ h_{\text{surf}}(k_x, k_y) = v_F \mathbf{D} \cdot \hat{s} - \mu, \]  

(4)

where \( v_F \) is the Fermi velocity. In what follows, we implicitly consider Bi\(_2\)Se\(_3\). However, the arguments below are valid for all TI’s. For Bi\(_2\)Se\(_3\), it is shown that \( \mathbf{D} = (-k_x, k_y) \). The Dirac point is at \((k_x, k_y) = (0,0)\), which we call \( \Lambda_0 \) in this paper. The dispersion relation becomes \( E_k = v_F |k| - \mu \). The spin configuration on the Fermi surface is schematically illustrated in Fig. 1(a), where we assume \( \mu > 0 \) and focus only on the upper Dirac cone. The direction of spin and that of momentum are locked to each other. Thus the spin direction flips abruptly at \( \Lambda_0 \) when we trace the electronic states along the line \( \mathbf{L} \) as shown in Fig. 1(b). Thus the Dirac point may be a kink at \( \Lambda_1 = (\pi,0) \) and \( \Lambda'_1 = (-\pi,0) \) in the upper Dirac cone. The states at \( \Lambda_1 \) and that at \( \Lambda'_1 \) must be identical to each other because the two points are connected by a reciprocal vector. In other words, the topology of the Brillouin zone is the same as that of two-dimensional torus \( (T^2 = S^1 \times S^1) \). Although the energy of the two states are equal to each other, the spin direction of the two states are opposite to each other. In the effective theory, \( \Lambda_1 \) and \( \Lambda'_1 \) characterize the different electronic states. In real TI’s, the effective theory usually works well because electric states on the Dirac cone is absorbed into the bulk energy bands before reaching at the zone boundary.

The interface state between a TI and a FI is also approximately described by the effective Hamiltonian around the Dirac point in two dimension:

\[ h_{\text{TI/FI}}(k_x, k_y) = h_{\text{surf}}(k_x, k_y) + \mathbf{M} \cdot \hat{s}, \]  

(5)

where \( \mathbf{M} \) is the exchange potential in FI. Effects of the FI on the interface state are considered only through \( \mathbf{M} \). It is easy to show that the magnetic moment perpendicular to the two-dimensional plane, \( M_z \), gives rise to a gap energy at \( \Lambda_0 \). The magnetic moment parallel to the interface \( (M_x, M_y, 0) \), on the other hand, shifts the Dirac point from \( \Lambda_0 \) to \( (M_x/v_F, -M_y/v_F) \). In addition to this, the Fermi level stays at the Dirac point even in the presence of \((M_x, M_y, 0)\). The conclusions obtained by analyzing Eq. (5) seem to be valid for weak exchange potentials smaller than the gap size of TI.

However, the typical gap size in TI is 100 meV whereas the gap of FI is of the order of eV. Thus low-energy electronic states around the gap of TI should be studied using more realistic theoretical model.

### III. EFFECTS OF BAND ASYMMETRY AND LARGE MAGNETIC MOMENT OF TI

Let us consider a TI in three dimension under the exchange potential due to the magnetic moment in a FI. The Hamiltonian reads

\[ H = \left( \begin{array}{c} \begin{pmatrix} h_0 & \mathbf{d}(k) \cdot \hat{s} \end{pmatrix} \\ \mathbf{d}(k) \cdot \hat{s} - h_0 \hat{s}_0 \end{pmatrix}, \right) \]  

(6)

\[ h_0 = M_0 - B_1 k_z^2 - B_2 (k_x^2 + k_y^2), \]  

(7)

\[ \mathbf{d}(k) = (A_2 k_x, A_2 k_y, A_1 k_z), \]  

(8)

where \( M_0, A_1, A_2, B_1, \) and \( B_2 \) are material parameters. The wave number in \( x, y, \) and \( z \) directions are denoted by \( k_x, k_y, \) and \( k_z \), respectively. The Hamiltonian (6) is decomposed into two parts:

\[ H = H_0 + H', \]  

(9)

\[ H_0 = \begin{pmatrix} (M_0 - B_1 k_z^2)\hat{s}_0 & A_1 k_z \hat{s}_z \\ -A_1 k_z \hat{s}_z & -(M_0 - B_1 k_z^2)\hat{s}_0 \end{pmatrix}, \]  

(10)

\[ H' = \begin{pmatrix} -B_2 (k_x^2 + k_y^2)\hat{s}_0 & A_2 (k_x \hat{s}_x + k_y \hat{s}_y) \\ A_2 (k_x \hat{s}_x + k_y \hat{s}_y) & B_2 (k_x^2 + k_y^2)\hat{s}_0 \end{pmatrix}. \]  

(11)

To analyze interface electric state, we apply the transformation \( k_z \rightarrow i\kappa \) in \( H_0 \),

\[ H_0 = \begin{pmatrix} (M_0 + B_1 \kappa^2)i\hat{s}_0 & iA_1 \kappa \hat{s}_z \\ iA_1 \kappa \hat{s}_z & -(M_0 + B_1 \kappa^2)i\hat{s}_0 \end{pmatrix}. \]  

(12)

In Fig. 1(c), schematic band structures of Europium chalcogenides are illustrated. The band structures are generally asymmetric with respect to the Fermi level in these materials, which we consider through two parameters \( M_1 \) and \( M_2 \) with \( M_1 \neq M_2 \) as shown in Fig. 1(c). The horizontal line shows the Fermi energy of FI. The lowest band and the highest one are spin splitted due to the exchange potential. We assume that the middle bands are spin degenerate. We consider the large asymmetry of the band structures through the exchange

**FIG. 1.** (Color online) (a) The spin configuration of the Fermi surface. (b) The spin configuration on the line \( L \). (c) The schematic band structure of a ferromagnetic insulator. The arrow in a band denotes spin direction and the horizontal line shows the Fermi energy.

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Hamiltonian

\[ H_m = \begin{pmatrix} M_1 & 0 & 0 & 0 \\ 0 & -M_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{13} \]

where \( \alpha \) indicates the direction of the magnetic moment in FI and \( \mu_m \) represents the asymmetry in the band structure. In these definition, \( M_1 = M_2 \) and \( M_1 \neq M_2 \) describe the symmetric and asymmetric band structures, respectively. We assume that the correction for Hamiltonian of surface state in TI has same manner.

A. Perpendicular magnetic moment to plane

When the magnetic moment of FI is perpendicular to the junction plane, the exchange Hamiltonian for the surface state is

\[ H_m = \begin{pmatrix} M_1 & 0 & 0 & 0 \\ 0 & -M_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{15} \]

In usual FI’s, a relation \( M_i \gg M_0 \) holds. The Hamiltonian \( H_0 + H_m \) is decomposed into two \( 2 \times 2 \) matrices whose eigenvalues are \( E_i = (\tilde{M}_i - M_0)/2 \) with \( \tilde{M}_1 = M_1 + M_0 \) and \( \tilde{M}_2 = -M_2 + M_0 \). The eigenstates of \( H_0 + H_m \) can be expressed by

\[ \psi_1(k_1) = \begin{pmatrix} a_1(k_1) \\ b_1(k_1) \end{pmatrix}, \quad \psi_2(k_2) = \begin{pmatrix} 0 \\ a_2(k_2) \\ b_2(k_2) \end{pmatrix}. \tag{16} \]

The coefficients \( a_i \) and \( b_i \) satisfy

\[ \frac{a_i}{b_i} = -\frac{iD_i\kappa}{(\tilde{M}_i + M_0)/2 - B_i\kappa^2}, \tag{17} \]

where \( D_1 = A_1 \) and \( D_2 = -A_1 \). This Hamiltonian is equivalent to that of the surface state of a TI facing to vacuum by substituting \((\tilde{M}_i + M_0)/2 \) by \( M_0 \).

The imaginary wave number \( \kappa^\pm \) takes different forms depending on the sign of \( \tilde{M}_1 + M_0 \). For \( \tilde{M}_1 + M_0 > 0 \), \( \kappa \) has the similar form as it is in the TI/vacuum surface,

\[ \kappa^\pm_1 = \frac{A_1}{2B_1} \left( 1 \pm \sqrt{1 - \frac{2B_1(\tilde{M}_1 + M_0)}{A_1^2}} \right). \tag{18} \]

The eigenstate in this case can be described by

\[ \left( \begin{array}{c} a_i \\ b_i \end{array} \right) = \left( \begin{array}{c} D_i/A_1 \\ i \end{array} \right) (C_+e^{-\kappa_1^+z} + C_-e^{-\kappa_1^-z}), \tag{19} \]

with \( C_\pm \) being arbitrary constants. For \( \tilde{M}_1 + M_0 < 0 \), the wave number becomes

\[ \kappa^\pm_1 = \frac{A_1}{2B_1} \left( \sqrt{1 - \frac{2B_1(\tilde{M}_1 + M_0)}{A_1^2}} \pm 1 \right). \tag{20} \]

The eigenstate is given by

\[ \left( \begin{array}{c} a_i \\ b_i \end{array} \right) = C_+ \left( D_i/A_1 \right) e^{-\kappa_1^+z} + C_- \left( -D_i/i \right) e^{-\kappa_1^-z}. \tag{21} \]

For \( M_1 > 0, \tilde{M}_1 + M_0 > 0 \) always holds. Thus \( \kappa_1 \) takes Eq. (18). On the other hand, \( \tilde{M}_1 + M_0 \) can be either positive or negative even for \( M_2 > 0 \).

We first analyze weak exchange potential satisfying \( M_2 < 2M_0 \). The wave function of in this case is

\[ \left( \begin{array}{c} a_i \\ b_i \end{array} \right) = \left( \begin{array}{c} D_i/A_1 \\ i \end{array} \right) (C_i^+e^{-\kappa_i^+z} + C_i^-e^{-\kappa_i^-z}). \tag{22} \]

with \( C_i^\pm \) being the normalization constant. For simplicity, in what follows, we drop \( z \) dependence from the wave function. There are only two independent wave function for \( M_2 < 2M_0 \). The surface state is a superposition of \( \psi_1 \) and \( \psi_2 \) that are defined by

\[ \psi_1 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ i \end{array} \right) , \quad \psi_2 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ -1 \end{array} \right). \tag{23} \]

The total Hamiltonian \( H_0 + H' + H_m \) can be represented in this basis of \( \psi_i \) as

\[ H = \left( \begin{array}{cc} M_1 & 0 \\ 0 & -M_2 \end{array} \right) + \left( \begin{array}{cc} H_{11} & H_{12} \\ H_{21} & H_{22} \end{array} \right) \]

\[ = \left( \begin{array}{cc} M_1 & iv_F(k_x - i k_y) \\ -iv_F(k_x + i k_y) & -M_2 \end{array} \right). \tag{24} \]

\[ H_{ij} = \langle \psi_i | H | \psi_j \rangle \tag{25} \]

with \( v_F = A_2 \). The energy of the surface state is

\[ E = \frac{M_1 - M_2}{2} \pm \sqrt{\frac{(M_1 + M_2)^2}{4} + v_F^2k^2} \tag{26} \]

with \( k = \sqrt{k_x^2 + k_y^2} \). For weak exchange potential \( M_2 < 2M_0 \), the exchange potential in the \( z \) direction causes the gap, which is consistent with the previous theories. 

The asymmetry of the band structures gives a constant energy shift to the dispersion relation.

Next, we consider strong exchange potential satisfying \( M_2 > 2M_0 \). In this case, the straightforward calculation of the eigenfunction at the \( \Gamma \) point results in

\[ \psi_1 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ i \end{array} \right) , \quad \psi_2 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ i \end{array} \right) , \quad \psi_3 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ i \end{array} \right). \tag{27} \]

For convenience, we employ another basis as follows:

\[ \psi_1 = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 0 \\ i \end{array} \right) , \quad \psi_2 = \left( \begin{array}{c} 0 \\ 1 \end{array} \right) , \quad \psi_3 = \left( \begin{array}{c} 0 \\ 0 \end{array} \right). \tag{28} \]

The total Hamiltonian \( H_0 + H' + H_m \) in this representation reads

\[ H = \left( \begin{array}{ccc} M_1 & -iv_F(k_x - i k_y) & 0 \\ iv_F(k_x + i k_y) & -M_2 - B_2 k^2 & 0 \\ 0 & v_F(k_x + i k_y) & -M_2 + B_2 k^2 \end{array} \right). \tag{29} \]
with \( v_F = A_2/\sqrt{2} \). The energy dispersion can be derived from the eigenequation
\[
\chi^3 - 2M\chi^2 - (B_2^2 k^4 + 2v_F^2 k^2)\chi + 2MB_2^2 k^4 = 0,
\]
with \( \chi = E + M \). At the vicinity of \( \Gamma \) point, \( \chi(k) \) is approximately given by
\[
\chi(k) = a_0 + a_1 k^2 + a_2 k^4.
\]
Here, \( a_0 \) can be obtained easily by putting \( k = 0 \). We obtain two values:
\[
a_0 = 0, \quad 2M.
\]
For \( a_0 = 0, a_1 \) can be derived by putting the coefficients of \( k^4 \) and \( k^6 \) terms in Eq. (30) to be zero. Since \( M \gg M_0 \), \( a_1 \) and \( a_2 \) have simple expression
\[
a_1 = -\frac{v_F^2}{2M}B_2 \sqrt{1 + \frac{v_F^4}{4M^2 B_2^2}},
\]
\[
\simeq -\frac{v_F^2}{2M}B_2,
\]
\[
a_2 = -\frac{v_F^2}{4M^2 B_2}.
\]
Then the energy dispersions are approximately given by
\[
E(k) = -M_2 \pm B_2 k^2 \pm \frac{v_F^2}{2M} B_2 k^4.
\]
In the same way, we also obtain
\[
E(k) = M_1 + \frac{v_F^2}{M} k^2 - \frac{v_F^4}{2M^2} k^4,
\]
for \( a_0 = 2M \). For both \( a_0 = 0 \) and \( 2M \), the coefficient of \( k^2 \) and that of \( k^4 \) have opposite sign to each other. In addition, we can also predict that two minima of the dispersion go across the Fermi level and the interface becomes metallic for \( M > 2M_0 \).

### B. Parallel magnetic moment to plane

When the magnetic moment of FI is parallel to the junction plane, the Hamiltonian of the surface state at \( \Gamma \) point is \( H_0 + H_m \) with
\[
H_m = \begin{pmatrix} M\sigma_x + \mu_m \delta_0 & 0 \\ 0 & 0 \end{pmatrix}.
\]
Here, we assume that the magnetic moment is in the \( x \) direction. This does not loose the generality of argument below because the Hamiltonian is rotationally invariant in momentum space. Applying a unitary transformation, we obtain
\[
U^\dagger (H_0 + H_m) U = \begin{pmatrix} (M_0 + B_1 k^2)\delta_0 + \tilde{M} & -iA_1 k \sigma_x \\ -iA_1 k \sigma_x & -(M_0 + B_1 k^2)\delta_0 \end{pmatrix},
\]
\[
\tilde{M} = \begin{pmatrix} M_1 & 0 \\ 0 & -M_2 \end{pmatrix}.
\]
with
\[
U = \begin{pmatrix} (\delta_0 - i\delta_y)/\sqrt{2} & 0 \\ 0 & (\delta_0 - i\delta_y)/\sqrt{2} \end{pmatrix}.
\]

The eigenvectors can be expressed by
\[
\psi_1 = \begin{pmatrix} a_1(k) \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} a_2(k) \\ b_2(k) \end{pmatrix},
\]
where \( \tilde{M}_1 = M_0 + M \) and \( M_2 = M_0 - M \). The eigenvalues and eigenvectors can be calculated in the same way with the previous section.

When the exchange potential is weak \( M_2 < 2M_0 \), the eigenvectors are the eigenvalues \( E_i \) are
\[
E_1 = \frac{M_1}{2}, \quad E_2 = -\frac{M_2}{2}.
\]
Corresponding vectors are given by
\[
\psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\]

The total Hamiltonian \( H = H_0 + U^\dagger H' U \) becomes
\[
H = \frac{M_1 - M_2}{2} s_0 + \begin{pmatrix} M - v_F k_y & -i v_F k_x \\ i v_F k_x & -M + v_F k_y \end{pmatrix},
\]
where \( v_F = A_2 \) and \( 2M = M_1 + M_2 \). The energy dispersion is given by
\[
E = \frac{M_1 - M_2}{2} \pm v_F \sqrt{k_x^2 + (k_y - M/v_F)^2}.
\]

The Dirac point moves from the \( \Gamma \) point to \( (0, M) \), which is consistent with the effective theory in around the Dirac point. The asymmetry of the band structures, however, shifts the Fermi level from the Dirac point.

When the exchange potential is sufficiently large satisfying \( M_2 > 2M_0 \), the basis of the surface state becomes
\[
\psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \psi_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.
\]

The total Hamiltonian \( H = H_0 + H' + H_m \) in this basis results in
\[
H = \begin{pmatrix} M_1 - v_F k_x & -i v_F k_x/\sqrt{2} \\ i v_F k_x/\sqrt{2} & -M_2 + B_2 k^2 \end{pmatrix},
\]
with \( v_F = A_2 \).

By analyzing Eq. (49) in detail, we can conclude that (a) there are two Dirac cones in the whole Brillouin zone, (b) the asymmetry of band structure in FI with respect to the Fermi level may causes the separation of the interface state from the bulk band, and (c) three branches of surface states appear in the gap of FI. These conclusions can be confirmed in a simple case where we consider the dispersion relation along a line satisfying \( k_y = 0 \). At \( k_x = 0 \), three dispersion branches appear...
at the interface
\[ E_1 = M_1 - v_F k_y, \]
\[ E_2 = -M_2 - v_F k_y \sqrt{1 + (B_2^2/v_F^2)k_y^2}, \]
\[ E_3 = -M_2 + v_F k_y \sqrt{1 + (B_2^2/v_F^2)k_y^2}. \]
Near the \( \Gamma \) point, two branches \( E_1 \) and \( E_2 \) are almost parallel to each other. The remaining branch \( E_3 \) goes across \( E_1 \) and \( E_2 \). Therefore there are two Dirac points. For \( k'_y = k_y - (M_1 + M_2)/2v_F \), Eqs. (50) and (52) can be represented by
\[ E = \frac{M_1 - M_2}{2} \pm v_F k'_y, \]
where higher order terms for \( k^3 \) in Eq. (52) are ignored. The first term implies a asymmetry of the band structure of FI. Another Dirac point is obtained by Eqs. (51) and (52) in the same way:
\[ E = -M_2 \pm v_F k_y, \]
where higher order terms for \( k^3 \) in Eqs. (51) and (52) are ignored. The schematic illustration for positions of two Dirac points is shown in Fig. 2(c).

As we have discussed above, the asymmetry of band structure in FI removes the dispersion of the interface state from the bulk band. This causes more drastic modification of interface state in the presence of magnetic moment parallel to the interface plane. When \( M = (M_x, 0, 0) \), the magnetic moment shifts the Dirac point from \( \Lambda_0 \) in the Brillouin zone to a point \( D \) as shown in Fig. 2(a). Let us consider the spin configuration along a line that satisfies \( D \parallel M \) (Eq. (4)) and passes through the Dirac point \( D \). For \( M = (M_x, 0, 0) \), the line corresponds to the straight line \( L \) connecting \( \Lambda_2 \) and \( \Lambda'_2 \) as shown in Fig. 2(a). We note two key features of spin direction along the line: (i) \( \Lambda_2 \) and \( \Lambda'_2 \) are identical point to each other and (ii) the spin direction flips at \( D \). If the number of the Dirac point is one, spin direction at \( \Lambda_2 \) and \( \Lambda'_2 \) would be opposite to each other. This statement, however, contradict to (i). Therefore the number of Dirac point must be an even integer on \( \Lambda_2 - \Lambda'_2 \). Since \( D \) is a Dirac point, at least one extra Dirac point is necessary on \( \Lambda_2 - \Lambda'_2 \) [see Fig. 2(b)].

This conclusion above can be obtained in more general argument. The Dirac point can be regarded as the magnetic monopole in the momentum space. The Gauss integration in the first Brillouin zone becomes finite in the presence of the single monopole. This integration should coincide with the path integration of \( \mathbf{D}(\mathbf{k}) \) along the zone boundary. However, the integration along the boundary vanishes because of the relation \( \mathbf{D}(-\mathbf{k}) = -\mathbf{D}^\dagger(\mathbf{k}) \). Thus there must be extra monopoles in the Brillouin zone. According to this argument, the number of the Dirac points must be even number in the Brillouin zone. In Eq. (52), two Dirac points are expected in the present situation. The conclusions obtained by the analytical calculation are confirmed by numerical simulation in the next section.

IV. NUMERICAL RESULTS IN 3D

Let us consider a junction of TI and FI on three-dimensional tight-binding lattice as shown in Fig. 3(a). We describe the TI by using the two-band model as
\[ H_{TI} = \sum_{j,j'} \sum_k [\tilde{\epsilon}^\dagger_{k,j,1} c_{k,j,1}^\dagger + \tilde{\epsilon}_{k,j,2} c_{k,j,2}] \begin{bmatrix} \hat{\xi}_{TI} \hat{\xi}_{0} & A \cdot \hat{s} \end{bmatrix} \begin{bmatrix} \tilde{\epsilon}_{k,j,1} \\ \tilde{\epsilon}_{k,j,2} \end{bmatrix}, \]
\[ \hat{\xi}_{TI} = \begin{bmatrix} M_0 - 2b_1 + 2b_2 \cos(k_x a) + 2b_2 \cos(k_y a) \\ -4b_2 - \mu_{TI} \delta_{j,j'} + b_1 (\delta_{j,j'+1} + \delta_{j,j'-1}) \end{bmatrix}, \]
\[ A = [a_2 k_x \delta_j, a_2 k_y \delta_j, -i a_1 (\delta_{j,j'+1} - \delta_{j,j'-1})], \]
where \( c_{k,j,v}^\dagger \) \((c_{k,j,v})\) is the creation (annihilation) operator of an electron with spin \( s \), belonging to the band \( v = 1 - 2, \ldots \)
having two-dimensional wave vector \( \mathbf{k} = (k_x, k_y) \), and at a lattice site \( j < 0 \) in the \( z \) direction. We used the periodic boundary condition in the \( xy \) plane.

In the same way, we describe the FI by

\[
H_{FI} = \sum_{j,j'} \sum_{k} \left[ \tilde{c}_{k,j,1} \tilde{c}_{k,j',2} \right]^\dagger \begin{pmatrix} (\xi_{FI} + E_1)\delta_0 & 0 \\ 0 & (\xi_{FI} + E_2)\delta_0 + \mathbf{M} \cdot \hat{s} \end{pmatrix} \begin{pmatrix} \tilde{c}_{k,j,1} \\ \tilde{c}_{k,j',2} \end{pmatrix},
\]

(59)

\[
\xi_{FI} = [2t \cos(k_x) + 2t \cos(k_y) - 8t - \mu_{FI}] \delta_{j,j'} + t(\delta_{j,j+1} + \delta_{j,j-1}).
\]

(60)

for \( j > 0 \). At the interface \( (j = 0) \), TI and FI are connected by

\[
H_I = \sum_k \left[ \tilde{c}_{k,0,1} \tilde{c}_{k,0,2} \right]^\dagger \begin{pmatrix} (\xi_I + E_1/2)\delta_0 & A' \cdot \hat{s} \\ A' \cdot \hat{s} & (-\xi_I + E_2/2)\delta_0 + \mathbf{M} \cdot \hat{s}/2 \end{pmatrix} \begin{pmatrix} \tilde{c}_{k,0,1} \\ \tilde{c}_{k,0,2} \end{pmatrix}.
\]

(61)

\[
2\xi_I = M_0 - 2b_1 + 2(b_2 + t) \cos(k_x) + 2(b_2 + t) \cos(k_y) - 4b_2 - 8t - \mu_{TI} - \mu_{FI}.
\]

(62)

\[
2A' = (a_2k_x, a_2k_y, 0).
\]

(63)

FIG. 4. (Color online) The global pictures of band structures are showed for a perpendicular (a) and a parallel (b) magnetic moments.

FIG. 5. (Color online) The band structures of TI/FI junction with a perpendicular (a) and (b) and parallel (c) and (d) magnetic moment are plotted of the energy \( E \) vs the wave vector \( k_y \). The optical gap of FI is locked in \( 2M_0 \) in (a) and (c). The magnitude of a magnetic moment of FI is \( 2M_0 \) and \( 5M_0 \). There are the surface band separated from the bulk band structure. The effect by shifting the Fermi energy in the optical gap is plotted in (b) and (d).
The hard-wall boundary condition along with $z$ axis is employed. The parameters in this calculation take values of $B_{12}S_{23}$: $a_1 = 7.86 M_0/a$, $a_2 = 14.6 M_0/a$, $b_1 = 3.57 \times 10 M_0/a^2$, and $b_2 = 2.02 \times 10^2 M_0/a^2$ in TI side. The lattice constant $a$ is about 5 Å. In FI, we assume $b_{FI} = 10^{-2} b_1$ and $E_1 = - E_2 = - M/2$. The total lattice size in the $z$ direction is 200 sites, where TI and FI occupy 150 and 50 sites, respectively. A schematic band picture of a FI is shown in Fig. 3(b). Electronic structure becomes asymmetric with respect to the Fermi level.

We first show the dispersion relations of the interface states rather large energy range for magnetic moment perpendicular to the interface [see Fig. 4(a)] and for magnetic moment parallel to the interface [see Fig. 4(b)], where the dispersion is calculated along $k_x = 0$, $\mu_{FI} = - M_0/2$, $M = 5 M_0$ in (a) and $M = 2 M_0$ in (b). The wave function of the interface states behaves like $e^{j b_0}$ for $j < 0$ in TI with $b_0$ being the inverse of localization in (b). In the figures, we also show the bulk band in TI. As we discussed in Sec. III, the upper dispersion in (a) is clearly separated from the bulk band of TI in whole Brillouin zone because of the band asymmetry in FI. The dispersions of the interface states for the magnetic moment parallel to the interface have rather complicated structure as shown in (b). We note that upper dispersion branch is well separated from the bulk band for $|k_x| > 0.3$. We zoom up the dispersion relations near the $\Gamma$ point and discuss their features in the next figures.

In Fig. 5(a), we show the dispersion relation of the interface states along $k_x = 0$ for the magnetic moment perpendicular to the interface. Here, we assume $\mu_{FI} = - M_0/2$ and show the results for $M = 2 M_0$ and $5 M_0$. When the magnetic moment is relatively small at $M = 2 M_0$, the Dirac cone disappears as predicted by the effective theory around the Dirac point. When we increase the exchange potential at $M = 5 M_0$, however, the dispersion of the interface state behaves like $\epsilon_k \approx \epsilon_0 - \alpha k^2 + \alpha k^4$. As a result, the interface states become metallic. Features of the metallic also depends on the Fermi level in the FI. The dispersion relation in Fig. 5(b) shows that the number of Fermi surface is one for $\mu_{FI} = M_0/2$, whereas for $\mu_{FI} = - M_0/2$ two Fermi surface appears. These numerical results are consistent with analytical ones in Sec. III.

Next, we look into the interface states at TI/FI junction in the presence of the magnetic moment parallel to the junction plane. Figure 5(c) shows the dispersion relation along $k_x = 0$ for $M \parallel x$, where $\mu_{FI} = 0$ and $M = 2 M_0$. There are two Dirac cones in the Brillouin zone, which is consistent with the argument in Sec. III. In Fig. 5(d), we show the results at $M = 2 M_0$ for $\mu_{FI} = - M_0/2$ and $M_0/2$. The characteristic features of the interface states are insensitive to parameters such as $\mu_{FI}$ and $M$. Finally, we show the energy dispersion for $\mu_{FI} = - M_0/2$ and $M = 2 M_0$ in two-dimensional Brillouin zone in Fig. 6(a). In this figure, it is clear that there are two Dirac points in two-dimensional Brillouin zone.

V. CONCLUSION

In this paper, we have studied electronic properties of interface state between a topological insulator (TI) and a ferromagnetic insulator (FI) by using two-band model in three-dimension in both analytically and numerically. The energy gap of FI is usually much larger than that of TI and the band structures in FI is asymmetric with respect to its Fermi level. The dispersion branches of the interface state are separated from the bulk band in whole Brillouin zone due to the asymmetry of the band structures. When the magnetic moment is in the perpendicular direction to the interface plane, the interface states become metallic. The number of Fermi surfaces of such interface states depends on the material parameters. When the magnetic moment is in the parallel direction to the interface plane, metallic states always appear irrespective of the amplitude of the exchange potential. The number of the Dirac point becomes even integers in whole Brillouin zone. Such drastic effects of the magnetic moment on interface states obtained in analytical calculation have been confirmed by the numerical simulation on the tight-binding lattice.

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