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Interface induced states at the boundary between a $3D$ topological insulator and a normal insulator

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We show that, when a three-dimensional ($3D$) narrow-gap semiconductor with inverted band gap ("topological insulator", TI) is attached to a $3D$ wide-gap semiconductor with non-inverted band gap ("normal insulator", NI), two types of bound electron states having different spatial distributions and spin textures arise at the TI/NI interface. Namely, the gapless ("topological") bound state can be accompanied by the emergence of the gapped ("ordinary") bound state. We describe these states in the framework of the envelope function method using a variational approach for the energy functional; their existence hinges on the ambivalent character of the constraint for the envelope functions that correspond to the "open" or "natural" boundary conditions at the interface. The properties of the ordinary state strongly depend on the effective interface potential, while the topological state is insensitive to the interface potential variation.

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Introduction. It was predicted [1, 2] that certain $3D$ semiconductors with strong spin-orbit coupling (SOC) and an inverted order of energy bands near some high-symmetry points in the Brillouin zone would have gapped electron states in the bulk, but gapless and spin-momentum locked surface states with the two-dimensional ($2D$) Dirac-like spectrum inside the bulk gap. An existence of these states, the properties of which are topologically protected by time-reversal symmetry, is the very fingerprint that distinguishes such the semiconductors, called the $3D$ topological insulators (TIs), from their topologically trivial counterparts, below called normal insulators (NIs).

Angle-resolved photo-emission spectroscopy experiments on a number of materials such as, for example, Bi_2Se_3 and Bi_2Te_3 or $TlBiSe_2$ have proven the existence of the mid-gap surface helical states with nearly linear low-energy spectrum [3–6]. When the $3D$ TI has a free surface, i.e. an interface with vacuum, it shows the aforesaid remarkable features of the topologically robust surface states, which can host a great deal of quantum transport phenomena [7–10]. However, for practical applications, one often requires multiple interfaces or channels rather than a single surface. It was predicted that the topological electron states have also to exist at the TI/NI interface [11]. In Ref. [11], using density functional theory to design superlattice structures based on Bi_2Se_3, it was shown that an interface state with an ideal Dirac cone is caused by alternating NI and TI. Recently Berntsen et al. have directly observed the Dirac states at the $Bi_2Se_3/Si(111)$ buried interface [12]. Another photoemission study [13] revealed an existence of interface topological states in the layered bulk crystal $(PbSe)_5(Bi_2Se_3)_{3m}$, which forms a natural multilayer heterostructure composed of TI and NI. The evidence of a large shift of the Dirac point towards the conduction band edge relative to the vacuum interface, due to the In_2Se_3 capping layer on epitaxial Bi_2Se_3 thin film, was reported in [14] demonstrating the possibility of controlling the Dirac cone in TI-based systems. The magneto-transport signatures of the opening of a magnetic gap in the spectrum of interface states due to broken time-reversal symmetry in hybrid GdN/Bi_2Se_3 heterostructure were detected in Ref. [15].

So the topological states can occur not only on the free surface of a $3D$ TI but also at the TI/NI interface. On the other hand, it is well known [16, 17] that ordinary electron states (bound or resonance) may also arise at the interface formed by two different semiconductors, even without a special requirement to their band in-

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version. Many of the proposed applications require an appropriate interface formed by a TI with another material, thus it is important to explore if and to what extent the electronic properties of a TI are modified by the TI/NI interface potential. In this letter, we show that two different types of in-gap bound states, topological and ordinary ones, exist at the TI/NI interface. Recently, we discussed a similar problem of a coexistence of the topological and ordinary ("convenient") electron states induced by a ferromagnetic δ layer embedded into a $3D$ TI [18]. Here, within the $\mathbf{k}\cdot\mathbf{p}$ approximation, we investigate the energy spectra and the envelope functions for these topologically different states on the TI side of the TI/NI interface. We concentrate only on the key aspects of the phenomenon omitting the cumbersome details of analytical calculations.

Model Hamiltonian and effective energy functional within the $\mathbf{k}\cdot\mathbf{p}$ method. To approximately describe the band electron states of a bulk semiconductor, $|n\mathbf{k}\rangle$ ($\mathbf{k}$ is a wave vector, n is a band index), in the region of the Brillouin zone around the point of band extrema $\mathbf{k}_0$, the $\mathbf{k}\cdot\mathbf{p}$ method is reputed to be adequate enough [19]. Under a perturbation smooth enough on the atomic scale, this method makes it possible to qualitatively predict evolution of the electron state wave function $\Psi_n(\mathbf{r})$ in terms of a product of a slowly varying envelope function $f_n(\mathbf{r})$ and the Bloch functions $|n\mathbf{k}_0\rangle = \exp(i\mathbf{k}_0\mathbf{r})u_{n\mathbf{k}_0}(\mathbf{r})$ of the unperturbed crystal at the point $\mathbf{k}_0$: $\Psi_n(\mathbf{r}) = f_n(\mathbf{r})|n\mathbf{k}_0\rangle$, $u_{n\mathbf{k}}(\mathbf{r})$ is the Bloch periodic function. The envelope function approach with generalized boundary conditions may also be applied to the description of localized and resonant interface states in the semiconductor junctions of different types, using Hermiticity and symmetry requirements (see, for example, [20]). It is evident that some information about the interface states is lost in this continual approach that is compensated for by its relative simplicity allowing a transparent description of the envelope functions and spectra.

We consider the TI/NI layered system with both the TI and NI layers treated as semi-infinite slabs joined at the interface, the boundary between the constituent materials is assumed to be perfectly flat. The system displays translational symmetry in the (x, y) interface plane located at $z = 0$. Let us denote by $\Theta(\mathbf{r})$ and $\Phi(\mathbf{r})$ the envelope functions for the TI half-space ($z > 0$) and the NI half-space ($z < 0$), respectively. An important point to note is that, in general case, the Bloch amplitudes of quantum states in the TI and NI bulks correspond to different irreducible representations of the different space groups of the crystal symmetry. So the envelope functions $\Theta(\mathbf{r})$ and $\Phi(\mathbf{r})$ (as well as their space derivatives) being defined on the different bases (u and w, respectively) do not keep continuity at the TI/NI interface.

The low energy and long wavelength bulk electronic states of the prototypical TI Bi_2Se_3 are described by the four band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian with strong SOC [21, 22]:

$$H_T(\mathbf{k}) = \varepsilon_0(\mathbf{k})\mathbf{I}_{4\times4} + \Xi(\mathbf{k})\tau_z\otimes\sigma_0 + \\ + A_{\parallel}(k_x\tau_x + k_y\tau_y)\otimes\sigma_x + A_z k_z\tau_x\otimes\sigma_z, \qquad (1)$$

where $\Xi(\mathbf{k}) = \Xi - B_{\parallel}(k_x^2 + k_y^2) - B_z k_z^2$; $\mathbf{I}_{4\times4}$ is an unit matrix, $\sigma_{0,x,y,z}$ and $\tau_{0,x,y,z}$ denote the Pauli matrices in the spin and orbital space, respectively. The Hamiltonian (1) is written in the basis $u = \{|+,\uparrow\rangle, |-,\uparrow\rangle, |+,\downarrow\rangle, |-,\downarrow\rangle\}$ of the four states at the Γ point with $\mathbf{k}_0 = 0$. The superscripts $\pm$ denote the even and odd parity states and the arrows $\downarrow\uparrow$ indicate the spin projections onto the z quantization axis. In the Bi_2Se_3-type materials, these four states originate from the bonding combinations of Bi $P1_z$-orbitals and anti-bonding combinations of Se $P2_z$-orbitals. The parameters Ξ, $B_{\parallel}$, B_z and $A_{\parallel}$, A_z are connected with matrix elements of momentum [22]. An important feature is that the orbitals $|+,\uparrow(\downarrow)\rangle$ and $|-,\uparrow(\downarrow)\rangle$ at the Γ point have the opposite parities, so that the off-diagonal terms are linear in $k_{\pm} = k_x \pm ik_y$ and k_z. The simple model (1) captures the remarkable features of the band structure, especially, under the condition Ξ, B_z, $B_{\parallel} > 0$, the inverted order of the energy terms $|+,\uparrow(\downarrow)\rangle$ and $|-,\uparrow(\downarrow)\rangle$ around $\mathbf{k}_0 = 0$ as compared with large $\mathbf{k}$, which correctly characterizes the topologically non-trivial nature of the system due to strong SOC. In what follows, without loss of generality we assume $\varepsilon_0(k) = 0$ and three-dimensional isotropy $B_z = B_{\parallel} = B$ and $A_z = A_{\parallel} = A$, which does not affect the topology. The dispersion of the bulk bands is given by $\omega(k) = \pm\sqrt{\Xi^2(k) + A^2k^2}$, $k = |\mathbf{k}|$.

The low energy and long wavelength bulk electronic states in NI are modeled by the four band Hamiltonian without SOC:

$$H_N(\mathbf{k}) = E_0(\mathbf{k})\mathbf{I}_{4\times4} + \Lambda(\mathbf{k})\tau_z\otimes\sigma_0, \qquad (2)$$

written in the basis $w = \{|c,\uparrow\rangle, |v,\uparrow\rangle, |c,\downarrow\rangle, |v,\downarrow\rangle\}$ which is constructed from the spin-degenerate states of the conduction band (c) and valence band (v) of the direct gap NI at the Γ point. For the sake of convenience we use a simple two-band effective mass approximation so that $\Lambda(\mathbf{k}) = \Lambda + Nk^2$, Λ, $N > 0$ and $E_0(\mathbf{k}) = E_0$; the electron and hole effective masses are implied to be the same, $m_{c,v} = (2N)^{-1}$. We regard NI as a wide-gap semiconductor in the sense that $|E_{c,v}| > \Xi$, where $E_c = E_0 + \Lambda$ and $E_v = E_0 - \Lambda$ are the edges of the corresponding bands.

We write the full electron energy of the TI/NI heterocontact in the following form:

$$\Omega = \int\limits_{z>0} d\mathbf{r}\Theta^{+}(\mathbf{r})H_T(-i\nabla)\Theta(\mathbf{r}) + $$

$$+ \int\limits_{z<0} d\mathbf{r}\Phi^{+}(\mathbf{r})H_N(-i\nabla)\Phi(\mathbf{r}) + \Omega_I, \qquad (3)$$

$$\Omega_I = \int d\mathbf{r}[\Theta^{+}(\mathbf{r})V(\mathbf{r})\Phi(\mathbf{r}) + \Phi^{+}(\mathbf{r})V^{+}(\mathbf{r})\Theta(\mathbf{r})]. \qquad (4)$$

Here, the operators $H_T(-i\nabla)$ and $H_N(-i\nabla)$ determined in Eqs. (1), (2) act in the space of the spinor functions $\Theta(\mathbf{r}) = [\theta_1(\mathbf{r}), \theta_2(\mathbf{r}), \theta_3(\mathbf{r}), \theta_4(\mathbf{r})]^{\mathrm{T}}$ and $\Phi(\mathbf{r}) = [\varphi^{(1)}(\mathbf{r}), \varphi^{(2)}(\mathbf{r}), \varphi^{(3)}(\mathbf{r}), \varphi^{(4)}(\mathbf{r})]^{\mathrm{T}}$ that are represented in the bases u and w, respectively. The components of the envelope functions $\Theta(\mathbf{r})$ and $\Phi(\mathbf{r})$ are smooth and continuous functions in the corresponding half-spaces. The spatial symmetry and periodicity of the heterostructure are broken due to the TI/NI interface. The $\mathbf{k}\cdot\mathbf{p}$ approach cannot provide information on the wave-function behavior in the vicinity of the atomically sharp interface, where large momenta are highly important. To overcome this serious drawback we introduce the effective potential of hybridization $V(\mathbf{r})$, which intermixes the electron states of the contacting constituents at the TI/NI interface. The hybridization $V(\mathbf{r})$ is nonzero in a small region d (of the order a lattice parameter) around the geometrical boundary $z = 0$, where the applicability of the $\mathbf{k}\cdot\mathbf{p}$ scheme is violated. The length d may be considered as an effective scale of the TI/NI interface region. An introduction of the phenomenological term of the interface energy Ω_I enables us to correctly reconcile the long-range variations of the electron density on both sides of the interface at $|z| > d$ in the terms of the boundary conditions for the envelope functions $\Theta(\mathbf{r})$ and $\Phi(\mathbf{r})$. As long as the spatial variations of the sought interface states are sufficiently slow, one can adopt a local approximation for the interface potential, namely, $V(\mathbf{r}) = dV(x,y)\delta(z)$, where $\delta(z)$ is the delta-function.

Next we make use a variational treatment for the energy functional

$$F\{\Theta^{+},\Theta,\Phi^{+},\Phi\} =$$

$$= \int\limits_{0+}^{\infty} dz\Theta^{+}(\boldsymbol{\kappa},z)[H_T(\boldsymbol{\kappa},-i\partial) - E]\Theta(\boldsymbol{\kappa},z) +$$

$$+ \int\limits_{-\infty}^{0-} dz\Phi^{+}(\boldsymbol{\kappa},z)[H_N(\boldsymbol{\kappa},-i\partial) - E]\Phi(\boldsymbol{\kappa},z) +$$

$$+ F_I\{\Theta^{+},\Theta,\Phi^{+},\Phi\}, \qquad (5)$$

$$F_I\{\Theta^{+},\Theta,\Phi^{+},\Phi\} = d[\Theta^{+}(\boldsymbol{\kappa},0+)V(\boldsymbol{\kappa})\Phi(\boldsymbol{\kappa},0-) +$$

$$+ \Phi^{+}(\boldsymbol{\kappa},0-)V^{+}(\boldsymbol{\kappa})\Theta(\boldsymbol{\kappa},0+)], \qquad (6)$$

where the energy E plays a role of the Lagrange multiplier. Since, in a plane geometry, the wave-vector $\boldsymbol{\kappa} = (k_x, k_y)$ is a good quantum number, we write the envelope functions in the mixed representation, $\Theta(\boldsymbol{\kappa},z)$ and $\Phi(\boldsymbol{\kappa},z)$, $\partial = \partial z$. The interface term $F_I\{\Theta^{+},\Theta,\Phi^{+},\Phi\}$ (6) (where $V(\boldsymbol{\kappa})$ is a 4×4 matrix) includes all possible components of hybridization between the TI states (1) and the NI states (2); $V(\boldsymbol{\kappa})$ is the Fourier transform of the function $V(x,y)$.

Varying functional $F\{\Theta^{+},\Theta,\Phi^{+},\Phi\}$ (5), (6) with respect to the functions Θ^{+} and Φ^{+} yields the Euler equations for the right ($z > 0$) and left ($z < 0$) half-spaces and the boundary conditions at the interface at $z = 0+$ and $z = 0-$, respectively. The relevant equations in the compact form are:

$$[H_T(\boldsymbol{\kappa},i\partial) - E]\Theta(\boldsymbol{\kappa},z) = 0, \qquad (7)$$

$$\text{either}\quad \delta\Theta^{+}(\boldsymbol{\kappa},0+) = 0$$

$$\text{or}\quad \Pi_T(\boldsymbol{\kappa},-i\partial)\Theta(\boldsymbol{\kappa},0+) - 2dV(\mathbf{k})\Phi(\boldsymbol{\kappa},0-) = 0, \qquad (8)$$

$$[H_N(\boldsymbol{\kappa},-i\partial) - E]\Phi(\boldsymbol{\kappa},z) = 0, \qquad (9)$$

$$\delta\Phi^{+}(\boldsymbol{\kappa},0-) = 0$$

$$\text{or}\quad \Pi_N(\boldsymbol{\kappa},-i\partial)\Phi(\boldsymbol{\kappa},0-) + 2dV^{+}(\mathbf{k})\Theta(\boldsymbol{\kappa},0+) = 0. \qquad (10)$$

It is convenient to express the boundary conditions in terms of the "current" density operator $\Pi_{T,N}(\boldsymbol{\kappa},k_z) = i\partial H_{T,N}(\mathbf{k})/\partial k_z$, which acts on the spinor functions $\Theta(\boldsymbol{\kappa},z)$ and $\Phi(\boldsymbol{\kappa},z)$. It is easy to see that the boundary conditions in Eqs. (8) and (10) lead to the "current" density conservation law:

$$\Theta^{+}(\boldsymbol{\kappa},z)\Pi_T(\boldsymbol{\kappa},-i\partial)\Theta(\boldsymbol{\kappa},z)|_{z=0+} -$$

$$- \Phi^{+}(\boldsymbol{\kappa},z)\Pi_N(\boldsymbol{\kappa},-i\partial)\Phi(\boldsymbol{\kappa},z)|_{z=0-} =$$

$$= 2F_I\{\Theta^{+},\Theta,\Phi^{+},\Phi\}. \qquad (11)$$

This equation means that the difference of the "currents" from the bulk to the interface (or vice versa) is exactly compensated by mutual transformations of the envelopes $\Theta(\boldsymbol{\kappa},z)$ and $\Phi(\boldsymbol{\kappa},z)$ due to the hybridization of the states u and w at the interface. In our model, the term F_I (6) plays a role of the "currents" source (sink) at the interface. It should be emphasized that the variational treatment provides two distinct options for the boundary conditions at the interface and, accordingly, two distinct interpretations of Eq. (11). On the one hand, we can strictly fix magnitude of the envelope functions at the interface, $\Theta(\boldsymbol{\kappa},0+) = 0$ and $\Phi(\boldsymbol{\kappa},0-) = 0$, then the partial "current" densities on both sides vanish at $z = 0$. This case corresponds to the so-called open boundary conditions [23]. On the other hand, we can put the constraint at $z = 0$ which connects the space derivatives and magnitudes of the envelope functions on the opposite sides of the interface following Eq. (8). This corresponds to the so-called natural boundary conditions [24]. To our knowledge, the ambivalence in the choice of boundary conditions has been formally discussed in Ref. [25] for the edge states of TI with an ideal free boundary.

Topological bound state at the interface. In accordance with Eqs. (9), (10), under the open boundary conditions at the interface, $\Phi(\boldsymbol{\kappa}, 0-) = 0$, and the decaying asymptotic far from it, $\Phi(\boldsymbol{\kappa}, z \to -\infty) = 0$, the envelope function in all the left half-space can be solely trivial, $\Phi(\boldsymbol{\kappa}, z) = 0$. In turn, the common solution of Eq. (7) for the envelope function in the right half-space satisfying the condition $\Theta(\boldsymbol{\kappa}, z \to \infty) = 0$ can be represented as

$$\theta_j(\boldsymbol{\kappa}, z) = a_j(\boldsymbol{\kappa}, E)\exp[-q_1(\kappa, E)z] + \\ + b_j(\boldsymbol{\kappa}, E)\exp[-q_2(\kappa, E)z], \quad (12)$$

where the characteristic momenta $q_{1,2}(\kappa, E)$

$$q_{1,2}(\kappa, E) = \frac{1}{\sqrt{2B}} \times \\ \times \left[A^2 - 2B\Xi(\kappa) \pm \sqrt{A^4 - 4B\Xi A^2 + 4B^2E^2}\right]^{1/2}, \quad (13)$$

are the roots of corresponding secular equation and $\kappa = |\boldsymbol{\kappa}|$. The boundary conditions at the TI/NI surface determine the expressions for $a_j(\boldsymbol{\kappa}, E)$ and $b_j(\boldsymbol{\kappa}, E)$.

Let us designate the envelope functions on the TI and NI sides satisfying the open boundary conditions as $\Theta_t(\boldsymbol{\kappa}, z)$ and $\Phi_t(\boldsymbol{\kappa}, z)$, respectively. Unlike the NI half-space ($z < 0$) with the normal band spectrum where $\Phi_t(\boldsymbol{\kappa}, z) \equiv 0$, near the boundary of the semiconductor with inverted gap ($z > 0$), the quasi-particle bound state with nontrivial envelope function $\Theta_t(\boldsymbol{\kappa}, z)$ exists even when the open boundary conditions are imposed on it. Indeed, as it has been shown in the work [23], the spinor function

$$\Theta_t^{(\pm)}(\boldsymbol{\kappa}, z) = \\ = C_t^{(\pm)}(\boldsymbol{\kappa})\Theta^{(\pm)}(\phi)\{\exp[-q_1^0(\kappa)z] - \exp[-q_2^0(\kappa)z]\}, \quad (14)$$

satisfies Eq. (7) under the condition $\Theta(\boldsymbol{\kappa}, 0+) = 0$. The function $\Theta_t^{(+)}(\boldsymbol{\kappa}, z)$ (14) describes the solution of the eigen state problem with the open boundary conditions for positive energy $E_t^{(+)}(\kappa) = |A|\kappa$, while the function $\Theta_t^{(-)}(\boldsymbol{\kappa}, z)$ (14) describes the state for negative energy $E_t^{(-)} = -|A|\kappa$; $\Theta^{(\pm)}(\phi) = (i, \mathrm{sgn}(A), \pm e^{i\phi}, \pm \mathrm{sgn}(A) i e^{i\phi})^{\mathrm{T}}$, $\phi = \phi(\boldsymbol{\kappa})$, $k_\pm = \kappa e^{\pm i\sigma\phi}$, $C_t^{(\pm)}(\boldsymbol{\kappa})$ are the normalization factors, and $q_{1,2}^0(\kappa) = q_{1,2}[\kappa, E_t^{(\pm)}(\kappa)]$ so that $q_1^0(\kappa) + q_2^0(\kappa) = |A|/B$. The momenta $q_{1,2}^0(\kappa)$ are either real quantities or complex conjugate ones. Correspondingly, if $A^2 > 4B\Xi(\kappa)$ the envelope functions (14) decay exponentially far away from the surface on the length of the order of $[q_{1,2}^0(\kappa)]^{-1}$, whereas if $A^2 < 4B\Xi(\kappa)$ the decay is accompanied by oscillations (below we restrict ourselves to the regime $A^2 > 4B\Xi$). Because the state (14) is induced by the transition from topological (TI) to trivial (NI) phase across the interface and is not influenced by the interface potential, we will consider it as the interface topological state. The spatial behavior of the envelope $\Theta_t^{(\pm)}(\boldsymbol{\kappa}, z)$ near the interface on the TI side is fully consistent with the trivial envelope $\Phi(\boldsymbol{\kappa}, z) = 0$ in the whole NI half-space. Thus, in the TI/NI heterostructure, the in-gap bound state is specified by the Dirac spectrum $E_t^{(\pm)}(\kappa) = \pm|A|\kappa$, $|E_t^{(\pm)}(\kappa)| < \Xi$, and the envelope function $\Theta_t^{(\pm)}(\boldsymbol{\kappa}, z)$ (14) at $z > 0$ and $\Phi_t(\boldsymbol{\kappa}, z) = 0$ at $z < 0$. However, this state is not a unique extremal of the functional (5), (6) on the class of piecewise smooth in both half-spaces and square integrable functions.

Ordinary bound state at the interface. Next we turn to the study of the extremal of the functional (5), (6) under the natural boundary conditions. Let us designate the envelope functions on the TI and NI sides satisfying the natural boundary conditions as $\Theta_0(\boldsymbol{\kappa}, z)$ and $\Phi_0(\boldsymbol{\kappa}, z)$, respectively. In accordance with Eqs. (9), (10), the envelope function $\Phi_0(\boldsymbol{\kappa}, z)$ is given by the exponential dependence

$$\varphi^{(n)}(\boldsymbol{\kappa}, z) = \varphi^{(n)}(\boldsymbol{\kappa}, 0)\exp[p^{(n)}(\kappa, E)z], \\ \varphi^{(n)}(\boldsymbol{\kappa}, 0) = \frac{(-1)^{n+1}d}{Np^{(n)}(\kappa)}\sum_{j=1}^{4} V_j^{(n)^*}(\boldsymbol{\kappa})\theta_j(\boldsymbol{\kappa}, 0), \quad (15)$$

where $p^{(n)}(\kappa, E) = \sqrt{\kappa^2 + [\Lambda + (-1)^{n+1}(E_0 - E)]/N}$, $V_j^{(n)}(\boldsymbol{\kappa})$ are the matrix elements of the effective potential of hybridization, the subscript j is related to the TI states, while the superscript (n) is related to the NI states. Then inserting Eq. (15) into Eq. (8) one can rewrite the latter in the following form:

$$\Pi_T(\boldsymbol{\kappa}, -i\partial)\Theta(\boldsymbol{\kappa}, 0) - 2dU(\mathbf{k}, E)\Theta(\boldsymbol{\kappa}, 0) = 0, \quad (16)$$

$$U_{jj'}(\boldsymbol{\kappa}, E) = \sum_{n=1}^{4}(-1)^{n+1}U_{jj'}^{(n)}(\boldsymbol{\kappa}, E), \\ U_{jj'}^{(n)}(\boldsymbol{\kappa}, E) = \frac{dV_j^{(n)}(\boldsymbol{\kappa})V_{j'}^{(n)^*}(\boldsymbol{\kappa})}{Np^{(n)}(\kappa, E)}. \quad (17)$$

Thus, under the natural boundary conditions, we reduce the problem to the search for the solution of Eq. (7) in the half-space $z > 0$, which satisfies the constraint conditions (16) at $z = 0$ containing an effective local (pseudo)potential $U(\boldsymbol{\kappa}, E)$ with the matrix elements $U_{jj'}(\boldsymbol{\kappa}, E)$ (17). Since the envelope function $\Theta_0(\boldsymbol{\kappa}, z)$ is strongly dominated by the interface perturbation (in contrast to the topological envelope function $\Theta_t(\boldsymbol{\kappa}, z)$), it is meaningful to call the relevant state as the ordinary interface state. Other feature of this state is nonzero magnitude of the envelope function on the NI side of the interface, $\Phi_0(\boldsymbol{\kappa}, 0) \sim \Theta_0(\boldsymbol{\kappa}, 0)$ (15).

In our model, the potential $U(\boldsymbol{\kappa}, E)$ occurs exclusively owing to the forbidding of a direct tunnelling of electron states over the interface, while the hybridization $V_j^{(n)}(\boldsymbol{\kappa})$ between the states of different symmetry at the interface is permitted. The matrix elements $U_{jj'}^{(n)}(\kappa, E)$ characterize internal properties of the TI/NI interface. Note, the sign of the diagonal matrix elements $U_{jj'}^{(n)}(\boldsymbol{\kappa}, E)$ (17) is predetermined ($U_{jj}^{(n)}(\boldsymbol{\kappa}, E) > 0$) so that the sign of $U_{jj}(\boldsymbol{\kappa}, E)$ depends on the contributions of relative intensities of the virtual electron transitions through the interface. Thereby, in the case of TIs like Bi_2Se_3, the parameters $U_{jj'}^{(n)}(\boldsymbol{\kappa}, E)$ should be chosen to distinguish between different possible terminating layers (Se or Bi) immediately adjacent to the interface. Let us descent to the particular case $V_1^{(n)}(\boldsymbol{\kappa}) = V_3^{(n)}(\boldsymbol{\kappa}) = 0$ and $V_2^{(n)}(\boldsymbol{\kappa}) \neq 0$, $V_4^{(n)}(\boldsymbol{\kappa}) \neq 0$. This choice corresponds with the plausible assumption that the orbitals of the topmost layer of the Bi_2Se_3 (111) composed of a Se layer (atomically flat surface over the whole interface area) dominantly contribute to the hybridization with the orbitals of NI. In such the case the effective potential $U(\kappa, E)$ (17) has four nonzero matrix elements: $U_{22}(\boldsymbol{\kappa}, E) = U_{44}(\boldsymbol{\kappa}, E) = P(\boldsymbol{\kappa}, E)$, $U_{24}(\boldsymbol{\kappa}, E) = U_{42}^*(\boldsymbol{\kappa}, E) = S(\boldsymbol{\kappa}, E)$. It is worth to note that the off-diagonal elements appear solely thanks to the spin-flip hybridization processes, which are presumed to be comparatively weak: $|S(\boldsymbol{\kappa}, E)| \ll |P(\boldsymbol{\kappa}, E)|$. In the following, for the sake of simplicity, we neglect the interface potential dependence on both $\boldsymbol{\kappa}$ and E.

By putting the trial solution (12) into the Eqs. (7) and (16), one obtains the set of equations for $a_j(\boldsymbol{\kappa}, E)$ and $b_j(\boldsymbol{\kappa}, E)$. After some algebra the corresponding secular equation results in the relation between the energy E and the in-plane momentum $\boldsymbol{\kappa}$ for the ordinary bound state at the interface, the expression for which is highly cumbersome. We will discuss only the main aspects of the corresponding spectrum dependence labeled by $E_0(\kappa)$. First, when the off-diagonal elements of the effective potential are absent, $S = 0$, the spectrum is approximately given by the quasi-linear dependence $E_0(\kappa) = E_0(0) + \alpha\kappa + \beta\kappa^2$ near the point $\kappa = 0$, where the parameters $E_0(0)$, α, and β are functions of the diagonal term P. It means that, due to the interface potential, the spectrum of the ordinary state, $E_0(\kappa)$, is entirely shifted and deformed as compared with the Dirac spectrum, $E_t^{(\pm)}(\kappa) = \pm|A|\kappa$, but it remains gapless. The node point of the spectrum $E_0(\kappa)$ is pinned to the energy $E_0(0)$ that is determined by the equation:

$$\left[1 - \sqrt{\frac{\Xi + E}{\Xi - E}}\right]\left[\frac{A^2}{4B} + \sqrt{\Xi^2 - E^2}\right] + $$
$$+ P\left[\frac{A^2}{B^2} + \frac{2}{B}(\sqrt{\Xi^2 - E^2} - \Xi)\right]^{1/2} = 0. \qquad (18)$$

The dependence of the node point position on the diagonal term P, $E_0(0) = h(P)$, for the given parameter of the TI bulk band structure $\lambda = A^2/4B\Xi$ is depicted in Fig. 1. If the term P is positive (negative) the node point

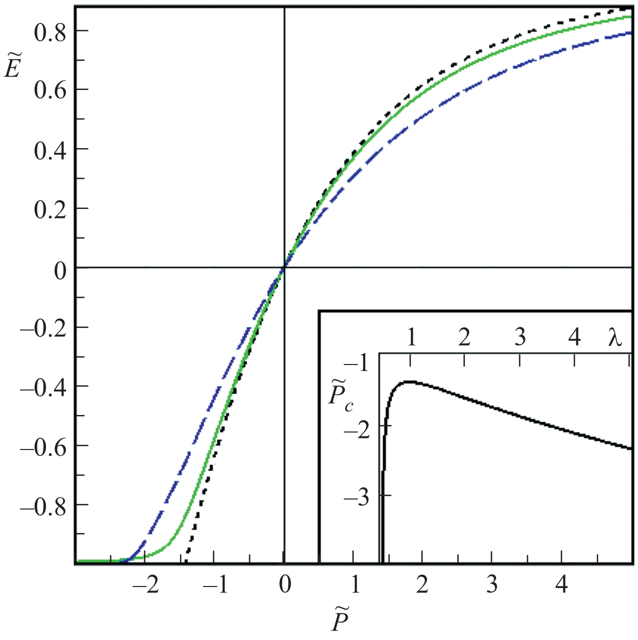

Fig. 1. (Color online) The bound state node position within the gap $\tilde{E} = E_0(0)/\Xi$ versus the effective surface potential $\tilde{P} = 2P/\sqrt{B\Xi}$ at given band parameter $\lambda = 0.5$ (green solid line), 1.0 (black dotted line), 5.0 (blue dashed line). Inset: dependence of the threshold value of $\tilde{P}_c$ on the band parameter λ

shifts towards the TI bulk conduction (valence) band edge. There is a threshold value, $P_c < 0$ ($h(P_c) = -\Xi$), so that for $P < P_c$ the node point leaves the gap for the bulk continuum. The plot $P_c(\lambda)$ is represented in the insertion in Fig. 1. When the interface potential is weak, $|P|/\Xi \ll 1$, we find the explicit expression for the upper and lower branches of the spectrum:

$$E_0^{(\pm)}(\kappa) = \pm|A|\kappa + \gamma(\kappa),$$
$$\gamma(\kappa) = dP\frac{|A|}{B}\Xi(\kappa)\left[\frac{A^2}{4B} + \Xi(\kappa)\right]^{-1}. \qquad (19)$$

Then for small momenta one has $E_0^{(\pm)}(\kappa) = \frac{2dP\sqrt{\Xi}}{\sqrt{B}}\frac{\sqrt{\lambda}}{1+\lambda} \pm |A|\kappa - \frac{2dP\sqrt{B}}{\sqrt{\Xi}}\frac{\lambda^{3/2}}{(1+\lambda)^2}\kappa^2$. The evolution of the spectrum $E_0^{(\pm)}(\kappa)$ as P is changed is schematically shown in Fig. 2. It is remarkable that,

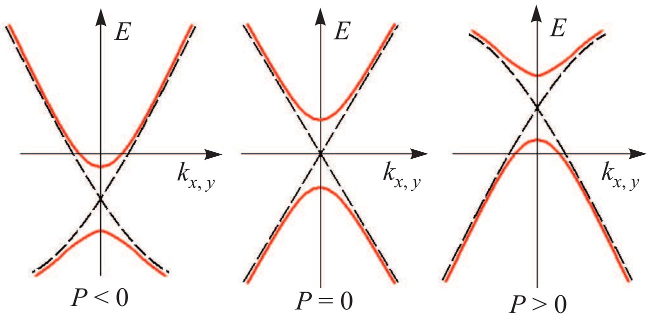

Fig. 2. (Color online) Schematic diagrams of the spectrum of the bound ordinary state evolving as a function of the interface potential without (black dashed line) and with (red solid line) spin-flip hybridization processes

when $P = 0$, the dependence (19) acquires the linear form $E_0^{(\pm)}(\kappa) = \pm|A|\kappa$, in other words, at $P = 0$ the energy spectrum for the interface states is independent of which boundary condition (open or natural) is chosen. In the limit $P \to 0$, the envelope function of the ordinary state, $\Theta_0^{(\pm)}(\boldsymbol{\kappa}, z)$, reduces to the rather simple form

$$\Theta_0^{(\pm)}(\boldsymbol{\kappa}, z) = C_0^{(\pm)}(\boldsymbol{\kappa})\Theta^{(\pm)}(\phi) \times$$
$$\times \{\exp[-q_1^0(\kappa)z] + \exp[-q_2^0(\kappa)z]\}, \qquad (20)$$

which differs from $\Theta_t^{(\pm)}(\boldsymbol{\kappa}, z)$ (14) only in sign of the second term in the braces. The space profile of the bound ordinary state depends strongly on P. For example, if the energy $E_0^{(\pm)}(\kappa)$ is near the bulk gap edge $\pm\Xi$, the envelope function $\Theta_0^{(\pm)}(\boldsymbol{\kappa}, z)$ is a superposition of two exponents of very different scales. The estimations of the relevant momenta are given by: $q_1(0) = \sqrt{2\Xi(2\lambda-1)/B}$ and $q_2(0) = \Xi\lambda/dP(2\lambda-1)$ when the states of TI and NI are strongly hybridized, $dP \gg \sqrt{B\Xi}$, or $q_2(0) = \Xi\lambda/d|P - P_x(\lambda)|(2\lambda-1)$ when the parameter P is close to the threshold value $P_c(\lambda)$. In principle we can obtain the envelope function $\Theta_0^{\pm}(\boldsymbol{\kappa}, z)$, at finite value $P \neq 0$. The analysis of its spinor form provided that the potential $U_{jj'}$ contains only the diagonal terms shows that the ordinary state has a nontrivial chiral spin structure: the direction of the spin-polarization vector is perpendicular to the electron momentum, $(\mathbf{s}(\kappa)\cdot\mathbf{k}) = 0$, besides the upper (lower) branch $\Theta_0^{(+)}(\boldsymbol{\kappa}, z)$ ($\Theta_0^{(-)}(\boldsymbol{\kappa}, z)$) with the energy above (below) the node $E_0(0)$ possess a left (right)-handed chirality. Such the behavior is similar to that of the topological state. The inclusion in consideration of the off-diagonal terms of the potential $U_{jj'}$ changes remarkably the properties of the ordinary bound state. The spin-flip hybridization processes $\sim S$ cause the energy gap opening at the node point: $|E_0^{(+)}(0) - E_0^{(-)}(0)| = |h(P+|S|) - h(P-|S|)|$, as shown in Fig. 2. Moreover in the case $S \neq 0$, the chiraliry of the ordinary state $\Theta_0^{(\pm)}(\kappa, z)$ is broken.

Conclusion. In summary, we have applied the envelope function method to study the in-gap bound states at the interface in the layered heterostructure, wherein the narrow-gap semiconductor with inverted band structure is in the contact with the wide-gap semiconductor with normal band structure. Within the framework of the variational procedure for the energy functional, we argue that both the open boundary conditions and the natural boundary conditions for the envelope functions are valid for this system. We have shown that two distinct types of the bound states appear at the interface, which are referred as the topological and ordinary states, respectively. The physical origin and properties of these states significantly differ from each other. The interface topological state stems from breaking the Z_2 invariant of TI [1, 2] at the boundary with NI. One emphasizes that, in the case of the heterocontact between different NIs, i.e., provided that $\Xi B < 0$ in the Hamiltonian (1), the nontrivial state satisfying the open boundary conditions does not exist. The main weight of the topological bound state does not occur at the interface, where $\Theta_t^{(\pm)}(\boldsymbol{\kappa}, 0) = 0$, but in the TI bulk region that is near the interface. Therefore, in our model, the interface induced topological state is insensitive to the local effective interface potential seen by electrons on the TI side. By contrast, the origin of the interface ordinary state is in one-to-one correspondence with the origin of the bound states of carriers due to the crystal symmetry breaking at the abrupt contact between different NIs in traditional semiconductor heterostructures [16, 17]. Since the maximum of the function $|\Theta_0(\boldsymbol{\kappa}, z)|$ takes place at the interface, the bound ordinary state is highly perceptive to the perturbations created by the coupling with NI.

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