Dirac-Fermion-Induced Parity Mixing in Superconducting Topological Insulators

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We self-consistently study surface states of superconducting topological insulators. We demonstrate that, if a topologically trivial bulk s-wave pairing symmetry is realized, parity mixing of pair potential near the surface is anomalously enhanced by surface Dirac fermions, opening an additional surface gap larger than the bulk one. In contrast to classical s-wave superconductors, the resulting surface density of state hosts an extra coherent peak at the induced gap besides a conventional peak at the bulk gap but no such surface parity mixing is induced by Dirac fermions for topological odd-parity superconductors. Our calculation suggests that the simple U-shaped scanning tunneling microscope spectrum in Cu₂Bi₂Se₃ does not originate from s-wave superconductivity, but can be explained by topological odd-parity superconductivity with a cylindrical Fermi surface.

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Introduction.— Topological superconductors (TSCs) are a new state of matter with nonzero topological numbers of bulk wave functions. The topologically protected gapless surface Andreev bound states (SABSs) are their own antiparticles, realizing Majorana fermions in condensed matter systems. Recently, the newly discovered superconductor Cu-doped Bi₂Se₃ has been considered as one potential TSC candidate. The parent material, Bi₂Se₃, is a topological insulator with gapless surface Dirac fermions, but superconductivity appears by intercalating Cu. The superconducting Cu₂Bi₂Se₃ retains the surface Dirac fermions in the normal state, and thus it is dubbed superconducting topological insulator (STI). From the Fermi surface structure of the material, Cu₂Bi₂Se₃ is predicted to be a TSC if time-reversal-invariant odd-parity superconductivity is realized.

Since TSCs predict gapless SABSs, tunneling spectroscopy via SABS can directly access the topological superconductivity. For Cu₂Bi₂Se₃, a point-contact experiment has revealed a pronounced zero-bias conductance peak (ZBCP) supporting a topological odd-parity superconductivity. The surface structure and tunneling spectroscopy have been studied theoretically, and the ZBCP of the experiment has been reproduced theoretically. There are also several other theoretical studies about this material.

Although similar ZBCPs have been observed independently, there also have been conflicting reports of tunneling spectroscopy recently. In particular, a scanning tunneling microscope (STM) experiment has indicated a simple U-shaped tunneling conductance for Cu₂Bi₂Se₃, which led to contrary statement that this material has a non-topological s-wave pairing symmetry.

In this Letter, we shall revisit surface states of STIs, motivated by the progress of experiments. Employing a self-consistent calculation, we shall clarify that the puzzling issue is understandable with the context of topological odd-parity pairing with the Fermi surface evolution. We also demonstrate that if non-topological s-wave pairing is realized in the bulk, the surface superconductivity is anomalously enhanced. Hence, the conventional s-wave pairing in Cu₂Bi₂Se₃ is accompanied by double coherence peaks in surface density of states (SDOS) but does not support a simple U-shaped SDOS.

Whereas there have been several theoretical works on the tunneling spectroscopy and the SDOS for STIs, the self-consistent analysis of the surface pairing potential has been lacking. In general, a subdominant pair potential could be induced near a surface by parity mixing of pair potential, since a surface breaks the bulk inversion symmetry. Moreover, for STIs, it is natural to expect that surface Dirac fermions may affect the surface superconductivity. It has been known from the study of high-Tc cuprates that, if such a subdominant pair potential exists, it could modify the SDOS and the resulting tunneling spectroscopy qualitatively.

Below, we show that, if an s-wave pairing is realized in the bulk, the pair potential is enhanced near the surface with a large parity mixing of the pairing symmetry. The enhanced pair potential opens a large gap for surface Dirac fermions, and thus the resultant SDOS hosts an extra coherent peak at the induced gap, in addition to a conventional peak at the bulk gap. We illustrate that the enhancement and the parity mixing are mediated by surface Dirac fermions in the normal state. We also examine surface states for bulk topological odd-parity pairing. In contrast to bulk s-wave pairing, neither mixture of a subdominant pair potential nor gap opening of surface Dirac fermions occurs. It is demonstrated that the Fermi surface evolution from spheroidal to cylindrical shape induces the topological phase transition. Based on our self-consistent analysis, therefore, the bulk topological pairing gives a consistent understanding on the ZBCP observed in Cu₂Bi₂Se₃.

Formalism.— We start with the Hamiltonian for STIs,
\( \mathcal{H} = \int d^3r \psi^\dagger_\alpha(r) [\mathcal{H}_{TI}(-i \nabla)]_{\alpha \beta} \psi_\beta(r) + \mathcal{H}_{\text{int}} \), proposed in Ref. [8], where \( \psi_\alpha \) and \( \psi^\dagger_\alpha \) are fermionic field operators, and the repeated Greek indices imply the sum over the orbital \( \sigma = 1, 2 \) and spin \( s = \uparrow, \downarrow \). For the single-particle Hamiltonian \( \mathcal{H}_{TI} \), we consider the following \( k \cdot p \) Hamiltonian describing the band structure of topological insulators near the \( \Gamma \) point:

\[
\mathcal{H}_{TI}(k) = c(k) + m(k) \sigma_x + v_z k_z \sigma_y + v_\sigma (k \times s)_z, \tag{1}
\]

where \( m(k) = m_0 + m_1 k_z^2 + m_2 (k_x^2 + k_y^2) \) with \( m_1, m_2 > 0 \) and \( c(k) = -\mu + c_1 k_x^2 + c_2 (k_x^2 + k_y^2) \) with the chemical potential \( \mu \). We introduce the Pauli matrices in the spin and orbital spaces, \( s_\mu \) and \( \sigma_\mu \). The interaction term is given by \( \mathcal{H}_{\text{int}} = \int d^3r [n^2_\uparrow(r) + n^2_\downarrow(r)] + 2vn_1(r)n_2(r)] \), where the electron density operator is defined as \( n_\sigma = \sum_r \psi^\dagger_\sigma(r) \psi_\sigma(r) \). Here, we consider intra- and inter-orbital density-density interactions \( U \) and \( V \).

The self-consistent electronic structure is obtained by solving the Bogoliubov-de Gennes equation \[ \mathcal{H}(-i \nabla) \varphi_I(r) = E_I \varphi_I(r), \tag{2} \]

where the eigenvector \( \varphi_I = (u_{1, \sigma}, x_1, u_{1, \sigma}, x_1, u_{1, \sigma}, x_1, u_{1, \sigma}, x_1)^T \) must satisfy the condition \( \int d^3r [\mathcal{H}(-i \nabla) \varphi_I(r)] \delta_{IJ} = \mathcal{H}_{TI}(-i \nabla) \).

The 4×4 matrix of the pair potential, \( \hat{\Delta} \), is obtained from

\[
i \begin{bmatrix} \Delta(r) s_y \end{bmatrix}_{\alpha \beta} = V_{\alpha \beta} \sum_{E_I > 0} [u_{I, \alpha}(r) u_{I, \beta}^*(r) f(E_I)
+ u_{I, \beta}(r) u_{I, \alpha}^*(r) f(-E_I)], \tag{4} \]

where \( V_{\alpha \beta} \) is \( U \) (V) for intra-orbital (inter-orbital) interactions and we set \( \alpha = (\sigma, s) \). We self-consistently solve Eqs. (2) and (4) with the discrete variable representation [38]. Corresponding to (111) surfaces of \( \text{Cu}_2\text{Bi}_2\text{Se}_3 \), which are naturally cleaved in the crystal of this material, we place the boundary condition \( \varphi_I(r) = 0 \) at \( z = 0 \) (bottom surface) and \( L \) (top surface). We assume homogeneity in the \( x-y \) plane parallel to the surface.

We set the parameters as \( m_0 = -0.28 \) eV, \( v_x = 3.09 \) eVÅ, \( v = 4.1 \) eVÅ, and \( \mu/m_0 = 1.8 \) [14, 17, 32]. The length scale is normalized with the coherence length \( \xi = v_F/\Delta_{\text{bulk}} \). The “Fermi velocity” of the conduction band is defined as \( v_F = 0 \text{E}_{\text{CB}}/\partial k_F \mid_{k_F} \), with the dispersion of the conduction band, \( E_{\text{CB}} = c_2 k^2 + \sqrt{m^2(k^2_x) + v^2 k^2_z} \), and the Fermi momentum \( k_F \) determined by \( E_{\text{CB}}(k_F) = \mu \), where \( k_0^2 = k^2_x + k^2_y \). Although we deal with the parameter range of \( m_1 \equiv m_1 m_0/v_x^2 \in [-0.17, -0.59] \) and \( \Delta_{\text{bulk}}/|m_0| \in [0.01, 0.1] \), here we present the results with \( m_1 = -0.17 \) and \( \Delta_{\text{bulk}} = 0.1 |m_0| \), which correspond to \( k_F \xi = 12.5 \). The separation between the conduction band and Dirac cone is quantified by \( \delta = (k_F^D - k_F)/k_F \) with the Fermi momentum of the Dirac cone \( k_F^D \). We find \( 0.05 < \delta < 0.18 \) for \(-0.033 < m_2 = m_2 m_0/v_x^2 < -0.33 \), consistent with Ref. [8]. We set \( T = 0 \) and \( V \) and \( V \) are chosen so as to fix the pair potential in the bulk, \( \Delta_{\text{bulk}} \).

Surface Dirac fermions of \( \text{Cu}_2\text{Bi}_2\text{Se}_3 \).— In Figs. (a) and (c), we show the energy spectra of \( \text{Cu}_2\text{Bi}_2\text{Se}_3 \) in the normal state. Like the parent topological insulator \( \text{Bi}_2\text{Se}_3 \), the topology of the normal state is characterized by the \( Z_2 \) invariant, \( \nu \), which obeys \( (1)^v = \text{sgn}(m_0 m_1) \).

For even \( \nu \)'s, topologically protected Dirac fermions are bound at the surfaces. As seen in Figs. (a) and (c), at the Fermi level of \( \text{Cu}_2\text{Bi}_2\text{Se}_3 \), the Dirac cone is well isolated from the bulk conduction band, which is consistent with angle-resolved photoemission spectroscopy data [8]. The separation \( \delta \) increases with decreasing magnitude of \( \delta \).

The wave function of Dirac fermions on the surface at \( z = 0 \) is solved for \( c_1 = c_2 = 0 \) as

\[
\varphi_D(z) = (e^{-k_\perp z} - e^{-k_\perp z}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes u_s(k_x, k_y), \tag{5} \]

with the boundary condition \( \varphi_D(0) = 0 \), where \( k_\perp \equiv v_z/2m_1 \pm \sqrt{(m_0 + m_2 k_0^2)/m_1 + (v_z/2m_1)^2} \) and \( (0, 1) \) is the spinor in the orbital space. The spinor \( u_s \) in spin space satisfies \( (k_x s_y - k_y s_x) u_s = s_y k_x u_s \) with \( s = \pm \). \( \varphi_D \) is localized near the surface for small \( k_\parallel \).

Interestingly, the wave function of Eq. (5) consists of only one orbital, i.e., \( \sigma = 2 \). In other words, surface Dirac fermions are fully polarized in the orbital space. This polarization is a consequence of the inversion sym-

![FIG. 1](image-url) (Color online) Energy spectra in the normal state with \( \Delta = 0 \) (a) and spatial profiles of \( \Delta_{\text{bulk}}(z) \) (b) for non-topological states for \( m_2 = -0.066 \) (\( \delta = 0.159 \)) and -0.20 (0.08) (c, d). “CB” and “VB” denote the conduction and valence bands, respectively. We set \( m_1 = -0.17 \).
metry breaking on a surface: In the bulk, the inversion symmetry, \( \mathcal{P}\mathcal{H}_T(k)\mathcal{P}^\dagger = \mathcal{H}_T(-k) \) (\( \mathcal{P} = \sigma_z \)), ensures the degeneracy in the orbital space, but on a surface, this symmetry is completely broken so that polarization can arise. As we will show below, the polarization has a significant influence on parity mixing and pairing symmetry near the surface.

Note that the \( c_1 \) and \( c_2 \) terms in Eq. (11) may weaken the orbital polarization of the Dirac cone. It turns out, however, that the effect of the \( c_1 \) and \( c_2 \) terms is negligible when \( \delta \) is fixed [27]. Thus, we set \( c_1 = c_2 = 0 \) below.

**Surface states of bulk s-wave pairing.**— We now turn to superconducting states. Because Fermi statistics requires \( \Delta \) to satisfy \( s_y \Delta^T s_y = \Delta \), there are six \( k \)-independent pairings in the bulk of Cu₃Bi₂Se₃ (\( \Delta_{1a} \), \( \Delta_{1b}\sigma_x \), \( \Delta_{2}\sigma_y s_z \), \( \Delta_{3}\sigma_z \), \( \Delta_{4x}\sigma_y s_x \), and \( \Delta_{4y}\sigma_y s_y \)), which are classified according to representations of the crystal point group \( D_{3d} \).

In the bulk, the short-range density-density interaction \( \mathcal{H}_{\text{int}} \) realizes either \( \Delta_{1a} + \Delta_{1b}\sigma_x \) or \( \Delta_{2}\sigma_y s_z \), depending on the model parameters \( U \) and \( V \). Whereas the former belongs to the trivial representation \( A_{1g} \) of \( D_{3d} \), corresponding to a topologically trivial s-wave pairing, the latter belongs to \( A_{1u} \), realizing a fully gapped topological odd-parity pairing.

Let us first consider the self-consistent surface state of the bulk \( A_{1g} \) pairing, that is, a topologically trivial s-wave pairing \( \Delta_{1a} \). For a while, we neglect the interorbital density-density interaction \( V \) for simplicity. Although the parity of the inversion is a good quantum number in the bulk, it can be mixed near a surface since a surface breaks the inversion symmetry. Hence, parity mixing of surface pair potential may occur, though the mixing pattern is restricted by symmetry surviving on the surface considered. For the (111) surface of Cu₃Bi₂Se₃, the mirror reflection in the \( y-z \) plane, \( \mathcal{M}_{yz} = i s_z \), restricts the possible mixing as

\[
\hat{\Delta}(z) = \Delta_{1a}(z) + \Delta_{3}(z)\sigma_z.
\]

The other pairings \( \Delta_{2} \), \( \Delta_{4x} \), and \( \Delta_{4y} \) cannot appear since they transform in a different manner than \( \Delta_{1a} \) under the mirror reflection. Note that for \( V \neq 0 \), the possible mixing of Eq. (6) is modified as \( \hat{\Delta} = \Delta_{1a} + \Delta_{1b}\sigma_x + \Delta_{3}\sigma_z \). As seen in Fig. S3 of Ref. [37], however, the induced \( \Delta_{1b} \) does not alter the double-peak structure of the SDOS.

Figures 1(b) and 1(d) show the self-consistently obtained pair potential of Eq. (2), for \( \tilde{m}_2 = -0.066 \) (\( \delta = 0.159 \)) and \(-0.20 \) (0.08), respectively. Whereas the pair potential consists of only the s-wave component \( \Delta_{1a} \) in the bulk, the surface at \( z = 0 \) induces a large mixing of the odd-parity pairing \( \Delta_{3} \). Moreover, the s-wave pairing \( \Delta_{1a} \) itself is strongly enhanced near the surface, being deviated from that of \( \Delta_{\text{bulk}} \). Both the mixing and the enhancement are strengthened by decreasing \( |\tilde{m}_2| \), i.e., by increasing \( \delta \), and they occur near the surface within the scale of the penetration depth of the Dirac cone, \( \ell \equiv \kappa^{-1} \ll \xi \).

The corresponding plots of local density of states (LDOS) \( N(z, E) \equiv \sum_\sigma N_\sigma(z, E) \) are shown in Figs. 2(a) and 2(b), where \( N_\sigma(z, E) = \sum_{I,s}|u_{I,s}^\sigma|^2 \delta(E - E_I) + |v_{I,s}^\sigma|^2 \delta(E + E_I) \). These figures clearly indicate the existence of an extra peak in the SDOS at \( E/\Delta_{\text{bulk}} \approx \pm 2.5 \) in Fig. 2(a) \( |E/\Delta_{\text{bulk}} \approx \pm 1.5 \) in Fig. 2(b)], in addition to the bulk coherent peak at \( E = \pm \Delta_{\text{bulk}} \). In Fig. 3(a), we display the averaged SDOS, \( \mathcal{N}(E) \equiv \int_{-\ell_0}^{\ell_0} N(z, E) dz \), where we set \( \ell_0 = 2k_F^{-1} \). The SDOS in the presence of surface Dirac fermions (Fig. 3(a)) sharply contrasts the SDOS of ordinary s-wave superconductors (see Fig. S5(c) in Ref. [37]): Whereas the SDOS of ordinary s-wave superconductors supports only the bulk coherent peak and thus it is simply U-shaped, the present SDOS is not because of the enhancement of the surface superconductivity due to parity mixing.

![FIG. 2: (Color online) LDOS \( N(z, E) \) of the \( A_{1g} \) state for \( \tilde{m}_2 = -0.066 \) (\( \delta = 0.159 \)) (a) and \(-0.20 \) (0.08) (b), where the pair potentials are shown in Figs. 1(b) and 1(d). The LDOS in \( \sigma = 1 \) and \( \sigma = 2 \) orbitals in the case of \( \tilde{m}_2 = -0.20 \) are shown in (c) and (d).](image)

![FIG. 3: (a) SDOS for the bulk s-wave pairing at \((\tilde{m}_1, \tilde{m}_2) = (-0.17, -0.20) \). (b) Comparison of spatial profiles of \( \Delta_{1a}(z) \) with \( V = 0 \) and \((\tilde{m}_1, \tilde{m}_2) = (-0.17, -0.066) \). In the solid curve, \( \Delta_3 \) is removed from the self-consistent iteration.](image)
Now we will propose a mechanism by which such anomalously large mixing and enhancement of surface pair potential can occur in STIs. The key is the orbital polarization of surface Dirac fermions and the parity mixing in Eq. (6): In Figs. 2(c) and 2(d), we decompose the LDOS of Fig. 2(b) into two orbital components $N_1$ and $N_2$. The decomposed LDOS clearly indicates that only the orbital $\sigma = 2$ contributes to the enhanced pair potential near the surface. This suggests that orbitally polarized surface Dirac fermions drive the enhancement of the pair potential. Note that the bulk quasiparticles cannot generate such a huge imbalance between $N_1$ and $N_2$, since they are degenerate in the orbital space.

Considering surface Dirac fermions, we can indeed explain the qualitative behaviors of the surface pair potential in Figs. 2(b) and 2(d): As was mentioned above, surface Dirac fermions are fully polarized in the $\sigma = 2$ orbital on the surface at $z = 0$. Therefore, near the surface, the $\sigma = 2$ component is dominated by surface Dirac fermions, whereas the $\sigma = 1$ component consists of only ordinary electrons from the bulk. This means that these two components can behave differently near the surface, and thus they determine the surface pair potential in different manners. In the $\sigma = 2$ component, a larger gap of surface Dirac fermions is favored to gain the condensation energy of Dirac fermions, but in the $\sigma = 1$ component, the surface pair potential should be smoothly connected to the bulk pair potential. As the $\sigma = 2$ ($\sigma = 1$) component of Eq. (6) is given by $\Delta_{1a} - \Delta_3 (\Delta_{1a} + \Delta_3)$, the former effect drives a nonzero surface parity mixing term $\Delta_3$ with a $\pi$ phase shift relative to $\Delta_{1a}$, and the latter gives the condition of $\Delta_{1a} + \Delta_4 \approx \Delta_{\text{bulk}}$, i.e., $\Delta_3 < 0$. The synergism between these two naturally leads to the enhancement of $\Delta_{1a} \approx \Delta_{\text{bulk}} + |\Delta_3|$ with a large parity mixing $\Delta_3$.

To substantiate the above argument, we demonstrate in Fig. 3(b) how the pair potential behaves if $\Delta_3$ is intentionally removed from the self-consistent iteration. This behavior clearly supports the notion that parity mixing is indispensable to the enhancement of the surface pair potential. Note also that the mixing and the enhancement of this mechanism should weaken as surface Dirac fermions are merged into the bulk, i.e., $\delta \rightarrow 0$. This is also consistent with the difference between Figs. 2(b) and 2(d) as well as that between Figs. 2(a) and 2(b).

Surface states of bulk odd-parity pairing. We also evaluate the self-consistent surface state for the bulk $A_{1u}$ state realizing a topological odd-parity superconductor. As illustrated in Fig. 3(a), the self-consistently determined pair potential shows neither parity mixing nor enhancement, in contrast to the case with $s$-wave pairing in Fig. 1. This is because being consistent with crystal symmetry on the surface prohibits parity mixing. The spatial dependence of the pair potential is merely a typical one in the presence of zero-energy SABSs [13, 41, 42]. The resulting SDOS in Fig. 3(b) is qualitatively the same as that in non-self-consistent calculations [14, 17]. Hence, the previous theoretical tunneling spectroscopy calculations, which are consistent with point-contact experimental data having ZBCP [14, 28, 30], are justified.

In Fig. 4(c), we plot the SDOS in the $A_{1u}$ state with a cylindrical Fermi surface, calculated from the tight-binding model on the hexagonal lattice (see Sec. S6 in Ref. [37]). This yields a simple U-shaped form even in the $A_{1u}$ state. This is because the time-reversal invariant point $\Gamma$ is not enclosed by the Fermi surface on the (111) axis [10, 11]. Therefore, the Fermi surface evolution from the spheroidal to cylindrical shape induces the topological phase transition. This feature is also observed in the case of $\Delta_{A_{1u}}$.

Concluding remarks. In summary, we have studied the self-consistent structure of STIs. We have found that, if the bulk pairing symmetry is of $s$-wave type, surface Dirac fermions induce a large magnitude of surface pair potential accompanied by parity mixing. As a result, the SDOS hosts an extra coherent peak at the induced gap as well as at the bulk gap. Since the anomalous enhancement of surface superconductivity is a direct consequence of well-isolated surface Dirac fermions and parity mixing through the subdominant pair potential, our theory is applicable equally to other STIs [43, 15].

The present result has a direct implication on a recent STM experiment on Cu$_2$Bi$_2$Se$_3$ [32]. Based on our theory, the classical U-shaped tunneling spectrum reported in Ref. [32] does not suggest an $s$-wave pairing of STI, contrary to the previous claim. Instead, we suggest here that the simple spectrum in Cu$_2$Bi$_2$Se$_3$ is related to the evolution of the Fermi surface reported recently [16]: We have demonstrated that no gapless SABS appears on the (111) surface even for the $A_{1u}$ odd-parity state, when the two-dimensional Fermi surface is realized in the bulk [10, 11]. At the same time, neither parity mixing nor enhancement of pair potential occurs for the $A_{1u}$ pairing in both two- and three-dimensional Fermi surfaces. Therefore, the two-dimensional odd-parity pairing naturally reproduces the simple U-shaped spectrum of

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{(Color online) Spatial profiles of pair potential (a) and SDOS (b) for the $A_{1u}$ odd-parity state with the separation $\delta = 0.08$. (c) SDOS in the $A_{1u}$ state with a cylindrical Fermi surface. The insets in (b) and (c) show the Fermi surface in the $k_x - k_z$ plane, where $a$ and $c$ are the lattice constants.}
\end{figure}
the STM experiment.

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[1] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[3] Y. Tanaka, M. Sato, and N. Nagaosa, J. Phys. Soc. Jpn. 81, 011013 (2012).
[4] J. Alicea, Rep. Prog. Phys. 75, 076501 (2012).
[5] F. Wilczek, Nature Phys. 5, 614 (2009).
[6] L. Fu and E. Berg, Phys. Rev. Lett. 105, 097001 (2010).
[7] Y. Ando, J. Phys. Soc. Jpn. 82, 102001 (2013).
[8] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[9] M. Z. Hasan and J. E. Moore, Ann. Rev. Cond. Mat. Phys. 2, 55 (2011).
[10] M. Sato, Phys. Rev. B 79, 214526 (2009).
[11] M. Sato, Phys. Rev. B 81, 220504(R) (2010).
[12] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. 74, 3451 (1995).
[13] S. Kashiwaya and Y. Tanaka, Rep. Prog. Phys. 63, 1641 (2000).
[14] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando, Phys. Rev. Lett. 107, 217001 (2011).
[15] L. Hao and T. K. Lee, Phys. Rev. B 83, 134516 (2011).
[16] T. H. Hsieh and L. Fu, Phys. Rev. Lett. 108, 107005 (2012).
[17] A. Yamakage, K. Yada, M. Sato, and Y. Tanaka, Phys. Rev. B 85, 180509 (2012).
[18] A. Yamakage, M. Sato, K. Yada, S. Kashiwaya, and Y. Tanaka, Phys. Rev. B 87, 100510(R) (2013).
[19] S.-K. Yip, Phys. Rev. B 87, 104505 (2013).
[20] T. Hashimoto, K. Yada, A. Yamakage, M. Sato, and Y. Tanaka, J. Phys. Soc. Jpn. 82, 044704 (2013).
[21] Y. Nagai, H. Nakamura, and M. Machida, ArXiv e-prints (2013), 1305.3025.
[22] B. Zocher and B. Rosenow, Phys. Rev. B 87, 155138 (2013).
[23] L. Chen and S. Wan, J. Phys.: Condens. Matter 25, 215702 (2013).
[24] A. M. Black-Schaffer and A. V. Balatsky, Phys. Rev. B 87, 220506(R) (2013).
[25] Y. Nagai, H. Nakamura, and M. Machida, to be published in JPSJ supplement (arXiv:1310.4934).
[26] P. M. R. Brydon, S. D. Sarma, H. -Y. Hui, and J. D. Sau, arXiv:1402.7061.
[27] J. Yuan, J.-H. Gao, W.-Q. Chen, F. Ye, Y. Zhou, and F.-C. Zhang, Phys. Rev. B 86, 104506 (2012).
[28] G. Koren, T. Kirzhner, E. Lahoud, K. B. Chashka, and A. Kanigel, Phys. Rev. B 84, 224521 (2011).
[29] T. Kirzhner, E. Lahoud, K. B. Chashka, Z. Salman, and A. Kanigel, Phys. Rev. B 86, 064517 (2012).
[30] G. Koren and T. Kirzhner, Phys. Rev. B 86, 144508 (2012).
Supplementary Material

S1. Gor’kov equation

In Sec. S1-S3, we explain the self-consistent equations which we have used in this letter. We start with the following Hamiltonian for spin-1/2 fermions with orbital degrees of freedom,

$$H = \int dr \psi_\alpha^\dagger(r) [H_{TT}(-i\nabla)]_{\alpha\beta}(r) \psi_\beta(r) + \frac{1}{2} \int dr_1 \int dr_2 V_{\alpha\beta}^{\gamma\delta}(r_{12}) \psi_\alpha^\dagger(r_1) \psi_\beta^\dagger(r_2) \psi_\gamma(r_2) \psi_\delta(r_1), \quad (S.1)$$

where $r_{12} = |r_1 - r_2|$ is the relative coordinate and $H_{TT}$ describes the effective Hamiltonian for doped topological insulators. The repeated Greek indices $\alpha, \beta, \delta, \gamma$ imply the sum over the orbital ($\sigma$) and spin ($s$) degrees of freedom of electrons: $\alpha \equiv (\sigma, s)$. The Matsubara Green’s functions are defined as

$$G(x_1, x_2) = \left( \frac{G(x_1, x_2)}{F(x_1, x_2)} \right) = \langle T_\tau [\Psi(x_1) \Psi^\dagger(x_2)] \rangle, \quad (S.2)$$

where $x_j \equiv (\tau_j, r_j)$ and $\langle \cdots \rangle \equiv \text{Tr}[e^{i(\Omega+\mu-N)/T} \cdots]$ with the thermodynamic potential $\Omega$. Here we have introduced the field operator in Nambu space as $\Psi = (\psi_{\sigma,\uparrow}, \psi_{\sigma,\downarrow}, \psi_{\sigma,\uparrow}^\dagger, \psi_{\sigma,\downarrow}^\dagger)^T$. Below, we expand $G$ by the Matsubara frequency $\omega_n = (2n + 1)\pi T$, $G(x_1, x_2) = T \sum_n G(r_1, r_2; \omega_n) e^{-i\omega_n r_{12}}$.

The Gor’kov equation is derived from the Heisenberg’s equation of motion for fermionic field operators, $\frac{d}{dt} \psi_\alpha(x_j) = [H, \psi_\alpha(x_j)]$, as

$$\int dr_3 [i\omega_n \delta(r_{13}) - \mathcal{H}(r_1, r_3)] G(r_3, r_2; \omega_n) = \mathcal{Z}_0 \delta(r_{12}), \quad (S.3)$$

where $\mathcal{H}$ is a $8 \times 8$ matrix in Nambu space,

$$\mathcal{H}(r_1, r_2) = \begin{pmatrix} \delta(r_{12})H_{TT}(-i\nabla) & -i\hat{\Delta}(r_1, r_2) s_y \\ i\hat{\Delta}^*(r_1, r_2) s_y & -\delta(r_{12})H_{TT}^*(i\nabla) \end{pmatrix}. \quad (S.4)$$

Here we have omitted the diagonal part of the self-energy matrix. The pair potential is defined by the anomalous Green’s functions,

$$\Delta_{\alpha\beta}(r_1, r_2) = -iV_{\alpha\beta}^{\gamma\delta}(r_{12}) [F(r_2, r_1; \tau_{12} = 0_+) s_y]_{\gamma\delta} = -i \lim_{\eta \rightarrow 0} T \sum_n V_{\alpha\beta}^{\gamma\delta}(r_{12}) [F(r_2, r_1; \omega_n) s_y]_{\gamma\delta} e^{-i\omega_n \eta}. \quad (S.5)$$

The Nambu-Gor’kov equation (S.3) and the gap equation (S.5) determine the pair potential in a self-consistent manner.

S2. Bogoliubov-de Gennes equation
Now we show that the Gor’kov equation is reduced to the Bogoliubov de Gennes (BdG) equation,

$$\int dr_2 \mathcal{H}(r_1, r_2) \varphi_I(r_2) = E_I \varphi_I(r_1). \quad (S.6)$$

Here the eigenvector $\varphi_I = (u_I, \sigma, v_I, \sigma, v_I, \sigma, v_I, \sigma, v_I, \sigma) \text{T}$ fulfills the orthonormal condition, $\int \varphi_I^\dagger(r) \varphi_J(r) dr = \delta_{IJ}$. We first note that the BdG Hamiltonian Eq. (S.4) is particle-hole symmetric, $\mathcal{C} \mathcal{H}(r_1, r_2) \mathcal{C}^{-1} = -\mathcal{H}(r_2, r_1)$, where $\mathcal{C} = \mathcal{Z} K$ with $K$ being the complex conjugation operator. The particle-hole symmetry of the BdG Hamiltonian ensures that the positive energy solution $\varphi_E(r)$ is associated with the negative energy solution $\varphi_{-E}(r) = \mathcal{C} \varphi_E(r)$. Therefore, the following $8 \times 8$ unitary matrix

$$u_I(r) \equiv [\varphi_I^{(1)}(r), \varphi_I^{(2)}(r), \varphi_I^{(3)}(r), \varphi_I^{(4)}(r), C\varphi_I^{(1)}(r), C\varphi_I^{(2)}(r), C\varphi_I^{(3)}(r), C\varphi_I^{(4)}(r)] \quad (S.7)$$

diagonalizes the BdG Hamiltonian as

$$\int dr_1 \int dr_2 u_I^\dagger(r_1) \mathcal{H}(r_1, r_2) u_I(r_2) = E_I, \quad (S.8)$$

with $E_I \equiv \text{diag}(E_I^{(1)}, E_I^{(2)}, E_I^{(3)}, E_I^{(4)}, -E_I^{(1)}, -E_I^{(2)}, -E_I^{(3)}, -E_I^{(4)})$. The unitary matrix $u_I(r)$ satisfies the orthonormal and completeness conditions, $\int u_I^\dagger(r_1) u_I(r_1) dr_1 = \delta_{I_1 I_2}$ and $\sum_I u_I(r_1) u_I^\dagger(r_2) = \delta(r_{12}) \mathcal{Z}$. By using the unitary matrix $u_I$, the solution of the Gor’kov equation (S.3) is obtained as,

$$G(r_1, r_2; \omega_n) = \sum_I \frac{u_I(r_1)}{i \omega_n - E_I} \frac{u_I^\dagger(r_2)}{i \omega_n + E_I}, \quad (S.9)$$

which can be recast into

$$G(r_1, r_2; \omega_n) = \sum_{E_I > 0} \left[ \varphi_I(r_1) \varphi_I^\dagger(r_2) + C \varphi_I(r_1) \varphi_I^\dagger(r_2) \mathcal{C}^{-1} \right] \frac{1}{i \omega_n - E_I + i \omega_n + E_I}. \quad (S.10)$$

From this expression, the sum over the Matsubara frequency in Eq. (S.5) results in the Fermi distribution function $f(x) \equiv 1/(e^{x/T} + 1)$, and thus, the gap equation is reduced to

$$i \left[ \hat{\Delta}(r_1, r_2) s_\alpha \right]_{\alpha\beta} = v^{\gamma\delta}_{\alpha\beta} \left( r_{12} \right) \sum_{E_I > 0} \left[ u_I, \delta(r_1) u_{I, \gamma}(r_2) f(E_I) + v^{\gamma}_{I, \delta}(r_1) u_{I, \sigma}(r_2) f(-E_I) \right]. \quad (S.11)$$

We solve the BdG equation Eq. (S.6) and the gap equation (S.11) self-consistently, instead of solving the Gor’kov equation directly.

S3. Gap equations for Cu$_2$Bi$_2$Se$_3$
In this letter, we consider the following short-range electron density-density interaction as pairing interaction of superconducting topological insulator Cu$_x$Bi$_2$Se$_3$:

$$\mathcal{H}_{\text{int}} = U \left[n_{1x}^2(r) + n_{2y}^2(r)\right] + 2Vn_1(r)n_2(r),$$

(S.12)

where the electron density operator in orbital $\sigma$ is defined as $n_\sigma = \sum_{s=\uparrow,\downarrow} \psi_{s,\sigma}^\dagger(r)\psi_{s,\sigma}(r)$, and $U$ and $V$ denote intra-orbital and inter-orbital interaction constant, respectively. The general form of the pairing interaction $\mathcal{V}_{\alpha\beta}^{\gamma\delta}(r_{12})$ in Eq. (S.11) is simplified to $\mathcal{V}_{\alpha\beta}^{\gamma\delta}(r_{12}) = \mathcal{V}_{\alpha\beta}\delta_{\alpha\delta}\delta_{\gamma\delta}(r_{12})$, where the intra-orbital interaction ($i.e.$, $\sigma_\alpha = \sigma_\beta$) yields $\mathcal{V}_{\alpha\beta} = U$ and the inter-orbital one ($\sigma_\alpha \neq \sigma_\beta$) gives $\mathcal{V}_{\alpha\beta} = V$. Using the effective pairing interaction, the gap equation (S.11) is recast into

$$i \left[\hat{\Delta}(r)s_y\right]_{\alpha\beta} = \mathcal{V}_{\alpha\beta} \sum_{E_I > 0} \left[u_{I,\alpha}(r)v_{I,\beta}^*(r)f(E_I) + v_{I,\alpha}^*(r)u_{I,\beta}(r)f(-E_I)\right].$$

(S.13)

with $\Delta_{\alpha\beta}(r_1, r_2) = \Delta_{\alpha\beta}(r_1)\delta(r_{12})$. The BdG equation (S.6) and gap equation (S.13) form a set of self-consistent equations for superconducting topological insulators.

The Fermi statistics of electrons imposes the condition $\hat{\Delta} = s_y\hat{\Delta}^T s_y$, on the pair potential $\hat{\Delta}$. There are six independent matrices, $(\Delta_{1a}, \Delta_{1b} \sigma_x, \Delta_{2} \sigma_y s_z, \Delta_{3} \sigma_z, \Delta_{4z} \sigma_y s_x, \Delta_{4y} \sigma_y s_y)$, that satisfy this condition [1, 4]. Hence, the general form of $\Delta(r)$ is expanded in terms of the six independent pairings

$$\hat{\Delta}(r) = \sum_j \Delta_j(r)\hat{\Gamma}_j,$$

(S.14)

Here the Hermitian matrices $\hat{\Gamma}_j = \hat{\Gamma}_j^\dagger$ ($j = 1a, 1b, 2, 3, 4x, 4y$) are given by, $\Gamma_{1a} = 1_{4\times 4}$, $\Gamma_{1b} = \sigma_x$, $\Gamma_{2} = \sigma_y s_z$, $\Gamma_{3} = \sigma_z$, $\Gamma_{4x} = \sigma_y s_x$, and $\Gamma_{4y} = \sigma_y s_y$, respectively. For the pair potential of Eq. (S.13), the coefficients $\Delta_j$ are calculated by $\Delta_j(r) = \frac{1}{\pi} \text{Tr}_4[\hat{\Gamma}_j \hat{\Delta}(r)]$.

In Table I, we summarize possible bulk pairing potentials of Cu$_x$Bi$_2$Se$_3$ and their properties.

S4. Numerical results: Surface states of bulk $s$-wave pairing

In this section, we present supplementary numerical data of self-consistently determined surface pair potential.
First, Fig. S1 illustrates how the surface pair potential depends on the separation of surface Dirac fermions from the bulk. The separation becomes worse from left [(a)] to right [(d)]. The first row of Fig. S1 shows the energy spectra in the normal state by solving \( \mathcal{H}_{TI}(-i \nabla) \varphi_D(r) = E \varphi_D(r) \), where the four-component vector \( \varphi_D(r) \) obeys the boundary conditions.

FIG. S1: (color online) The first row shows the energy spectra in the normal state for \( \tilde{m}_1 = -0.17 \) and various \( \tilde{m}_2 \): \( \tilde{m}_2 = -0.066 \) (\( \delta = 0.159 \)) (a), \( -0.133 \) (\( \delta = 0.118 \)) (b), \( -0.20 \) (\( \delta = 0.08 \)) (c), and \( -0.266 \) (\( \delta = 0.04 \)) (d). In the second (third) row, we plot the spatial profiles of the pair potentials in the vicinity of the surface, \( \Delta_{1a} \) and \( \Delta_3 \). Figures in the fourth row depicts the quasiparticle energy spectra for the superconducting \( \Delta_{1a} \) state (bulk s-wave pairing state). Here we set \( V = 0 \) and \( \Delta_{\text{bulk}} \equiv \Delta_{1a} \left( z = L/2 \right) = 0.1|m_0| \). The thick lines (blue color) show the dispersion originating from the surface Dirac fermions.
condition, $\varphi_D(r) = 0$, on the surfaces $z = 0$ and $z = L$. We assume uniform infinite $x$-$y$ plane. The wave function is factorized as $\varphi_D(r) = e^{ik_x x + ik_y y} \varphi_D(z)$. The effective Hamiltonian describing the band structure of Bi$_2$Se$_3$ near the $\Gamma$ point is

$$H_{TI}(k) = c(k) + m(k)\sigma_x + v_z k_z \sigma_y + v \sigma_z (k_x s_y - k_y s_x),$$

(S.15)

where $m(k) = m_0 + m_1 k_x^2 + m_2(k_x^2 + k_y^2)$ with $m_1 m_2 > 0$ and $c(k) = -\mu + c_1 k_x^2 + c_2(k_x^2 + k_y^2)$ with the chemical potential $\mu$. Here we set the parameters to be $m_0 = -0.28$ eV, $v_z = 3.09$ eV\AA, $v = 4.1$ eV\AA, and $m_1 = -5.80$ eV\AA and the chemical potential is fixed to be $\mu/|m_0| = 1.8$ [4, 5]. The parameter $m_2$ takes various values in the range of $\tilde{m}_2 = m_2/m_0/v_z^2 \in [-0.033, -0.33]$. The non-trivial topology of the normal state is characterized by the $\mathbb{Z}_2$ number $\nu$, which obeys the relation

$$(-1)^\nu = \text{sgn}(m_0 m_1).$$

(S.16)

In the case of odd $\nu$’s, the gapless Dirac cone exists, whose wave function is bound on the surfaces within the penetration depth $\ell \equiv \kappa^{-1}$ (see Eq. (6) and the subsequent sentences in the main text). To quantify the separation of the Dirac cone from the bulk conduction band, we introduce

$$\delta \equiv \frac{k_D^F - k_F^F}{k_F^F},$$

(S.17)

where $k_D^F$ is the Fermi momentum of the surface Dirac cone. We find $0.05 < \delta < 0.18$ for the range of $-0.033 < \tilde{m}_2 < 0.33$ for $\tilde{m}_1 = -0.17$, which is consistent with angle-resolved photoemission spectroscopy data [6]. As illustrated in the first row of Fig. S1, the surface Dirac cone is well isolated from the bulk spectrum at the Fermi level for small $|\tilde{m}_2|$.

In the second row of Fig. S1 we show corresponding numerical results of pair potentials near the (111) surface in the superconducting state. Here we have assumed $s$-wave pairing symmetry ($A_{1g}$ state of Table S1) in the bulk. The pair potentials are obtained by solving self-consistently the BdG equation (S.6) and gap equation (S.13) in zero temperature. We set $V = 0$, and $U$ is chosen so as to fix the pair potential in the bulk as $\Delta_{\text{bulk}} = 0.1|m_0|$, which corresponds to $k_F \xi = 12.5$ in terms of the coherence length $\xi = v_F/\Delta_{\text{bulk}}$ with “Fermi velocity” $v_F = \partial E_{\text{CB}}(k_F) / \partial k_F |_{k_F}$. The Fermi momentum of the conduction band, $k_F$, is determined by solving $E_{\text{CB}}(k_F) = \mu$, where $k_F^2 = k_x^2 + k_y^2$. The results in the second row clearly indicate that the odd-parity pairing $\Delta_3$ is induced in the surface region within the length scale of the penetration depth of the Dirac cone $\ell$. 
The third row of Fig. S1 decomposes the same pair potentials in the orbital components, \( \Delta_{1a}(z) \pm \Delta_{3}(z) \). It is seen that the pair potential \( \Delta_{1a} - \Delta_{3} \) for the \( \sigma = 2 \) orbital is strongly enhanced near the surface, while the pair potential \( \Delta_{1a} + \Delta_{3} \) for the \( \sigma = 1 \) orbital is not. This reflects that the surface Dirac fermions occupy only one orbital state, \( \sigma = 2 \) (see Eq. (6) in the main text).

The quasiparticle energy spectra in the bulk \( s \)-wave pairing state, \( E(k_x, k_y) \), are displayed in the fourth row of Fig. S1. The quasiparticle spectra have a two-gap structure, where a larger gap, \( E = \pm \Delta_{\text{surf}} \), opens for the surface Dirac fermions in addition to the bulk gap \( E = \pm \Delta_{\text{bulk}} \). The magnitude of the surface gap is enhanced with decreasing the amplitude of \( \tilde{m}_2 \).

In Figs. S2(a-d), we depict the local density of states (LDOS) for the self-consistent solutions displayed in Fig. S1. The LDOS is obtained from the analytic continuation of the Green’s function in Eq. (S.10) as

\[
N(r, E) = -\frac{1}{\pi} \text{Tr}_4 G(r, r; \omega_n \to -iE + 0+) ,
\]

where \( 0_+ \) is an infinitesimal constant. The LDOSs in the vicinity of the surface indicate that the surface Dirac fermions support an energy gap, \( \Delta_{\text{surf}} \), larger than \( \Delta_{\text{bulk}} \). The surface gap becomes larger with decreasing \( |\tilde{m}_2| \).

We have numerically checked how the surface pair potential behaves for weaker pairing \( k_F \xi \gg 1 \). Figure S4 shows the self-consistently obtained pair potentials for \( k_F \xi = 12.5, 50, \) and \( 125 \). It turns out that the parity mixing and the enhancement of the surface pair potential are robust for weak pairing.

Figures S3(a) and S3(b) illustrate the pair potentials and the LDOS for the bulk \( s \)-wave pairing state with a finite inter-orbital coupling \( V/U = 1.0 \). The inter-orbital spin-singlet pairing \( \Delta_{1b} \) is induced by nonzero \( V \) in the vicinity of the surface. Nevertheless, the SDOS does not alter the double-peak structure, as illustrated in Fig. S1(b).

For comparison, we have also studied the case without surface Dirac fermions. This case is realized by choosing a topologically trivial normal state with \( \text{sgn}(m_0 m_1) = +1 \). The resultant LDOS is shown in Fig. S3(c), which yields a

\[
(a) \quad \delta = 0.159 \quad (b) \quad \delta = 0.118 \quad (c) \quad \delta = 0.08 \quad (d) \quad \delta = 0.04
\]

FIG. S2: LDOSs in the bulk \( s \)-wave pairing state (the \( A_{1g} \) state) for \( \tilde{m}_1 = -0.17; \tilde{m}_2 = -0.066 \) \((\delta = 0.159) \) (a), \(-0.133 \) \((\delta = 0.118) \) (b), \(-0.20 \) \((\delta = 0.08) \) (c), and \(-0.266 \) \((\delta = 0.04) \) (d). The parameters are same as those in Fig. S1.
FIG. S3: (color online) Spatial profiles of the pair potentials in the non-topological s-wave pairing, \( A_{1g} \) state, for various \( k_{\mu}\xi \)'s: \( k_{\mu}\xi = 12.5, 15, \) and 125. We here set \( V = 0, \tilde{m}_1 = -0.17, \) and \( \tilde{m}_2 = -0.20 (\delta = 0.08) \). The solid and broken lines denote \( \Delta_{1a}(z) \) and \( \Delta_{3}(z) \), respectively. The subdominant pair potential and the enhancement of \( \Delta_{1a} \) on the surface are unchanged by increasing the dimensionless parameter \( k_{\mu}\xi \), where the deviation and enhancement of the pair potentials are tightly bound at the length scale of the penetration depth of the surface Dirac fermion, \( \ell \sim 2k_{\mu}^{-1} \).

merely simple U-shape even in the vicinity of the surface. This result supports our claim that the existence of surface Dirac fermions is indispensable to the large parity mixing and enhancement of the surface pair potential.

In Fig. S5 we discuss the effect of the diagonal self-energy \( c_1k_z^2 + c_2k_\parallel^2 \) in the \( A_{1g} \) state. The term coupled to \( c_2 \) changes the Fermi radius \( k_F \) of the conduction band at \( k_z = 0 \), while the \( c_1 \) term relatively shifts the Fermi momentum of the Dirac cone, as shown in Fig. S5(a). Note that for Bi\(_2\)Se\(_3\), the values of \( \tilde{c}_1 \) and \( \tilde{c}_2 \) are estimated as \(-0.3 \) and \(-1.6 \) \([9]\). However, the Dirac cone is ill-defined at the Fermi level if we use the same parameters given in Ref. \([9]\). The

FIG. S4: Spatial profile of pair potentials (a) and LDOS (b) for the bulk s-wave superconducting \( A_{1g} \) state with \( V/U = 1.0 \) and \((\tilde{m}_1, \tilde{m}_2) = (-0.17, -0.20) (\delta = 0.08) \). (c) LDOS for the bulk \( A_{1g} \) state with \( \hat{\Delta} = \Delta_1 \), where the underlying normal electrons are topologically trivial, i.e., \( \text{sgn}(m_0m_1) = +1 \), which is not accompanied by the surface Dirac fermion.
FIG. S5: (color online) (a) Energy spectra of the normal state for $\tilde{c}_1 = 0.0$, $-0.03$, and $-0.06$, where we set $\tilde{m}_1 = -0.17$, $\tilde{m}_2 = -0.066$, and $\tilde{c}_2 = -0.1$ are fixed. (b) Difference $\delta$ between the Fermi surfaces of the conduction band $k_F$ and the Dirac cone $k_F^D$ as a function of $\tilde{c}_1$ for $\tilde{c}_2 = 0.0$, $-0.1$, and $-0.2$. The inset in (c) shows $N_1(0)/N_2(0)$ for $(\tilde{c}_1, \tilde{c}_2) = (0,0)$ and $(-0.0052, -0.2)$, where $N_\sigma(0)$ is the zero-energy LDOS of the $\sigma$ orbital in the normal state.

well-defined surface Dirac cone requires $|\tilde{c}_1|$ and $|\tilde{c}_2|$ to be sufficiently small in addition to the small $\tilde{m}_2$.

The separation $\delta$ defined in Eq. (S.17) is plotted in Fig. S5(b) as a function of $\tilde{c}_1 = m_0 c_1 / v_z^2$ for various $\tilde{c}_2$. It is seen that as $|\tilde{c}_1|$ increases, the surface Dirac cone is merged to the bulk conduction band. To clarify the effect of the $\tilde{c}_1$ and $\tilde{c}_2$ terms on the enhancement of the pair potential at the surface, we plot the spatial profiles of the $\Delta_1 \pm \Delta_3$ for $(\tilde{c}_1, \tilde{c}_2) = (0,0)$ and $(0.0052, -0.2)$, where the separation is fixed to be $\delta = 0.159$. As seen in Fig. S5, the ratio of the surface density of states (SDOS) in each orbital is slightly deviated by increasing $|c_1|$ and $|c_2|$, which indicates that the relative population of the orbitals in the surface Dirac cone varies. The spatial profile of the pair potentials at the surface is, however, insensitive to the increase of $|c_1|$ and $|c_2|$.

Finally, using Eq. (S.18), we calculate the SDOS defined as

$$ N(E) = \frac{1}{l_0} \int_0^{l_0} N(z, E) dz, \quad (S.19) $$

which is a direct observable in STM experiments. The length scale $l_0$ denotes the probing depth and is of the atomic order $\sim k_F^{-1}$. In Fig. S6 we plot $N(E)$ for the bulk $s$-wave superconducting state with $k_F \xi = 125$, which clearly indicates an extra coherent peak at the surface gap $E = \pm \Delta_{\text{surf}} \approx 1.6 \Delta_{\text{bulk}}$, besides the conventional peak at the bulk gap. In contrast, such a double-peak structure is never seen in the case without the surface Dirac fermions (see Fig. S5(c)), where the electron state in the normal state is a topologically trivial, $\text{sgn}(m_0 m_1) = +1$.

S5. Surface states of bulk topological odd-parity pairing

We now turn to the results for bulk topological odd parity superconductor, $\hat{\Delta} = \Delta_2 \sigma_y s_z$. As shown in Fig. S7(a), the self-consistently determined pair potential is suppressed near the surface region and the subdominant component
FIG. S6: (color online) SDOS, $N(E)$, for the bulk s-wave superconducting states, where we set $k_F \xi = 125$, $(\tilde{m}_1, \tilde{m}_2) = (-0.17, -0.20)$, and $V = 0$ ($\delta = 0.08$). The definition for $N(E)$ is given in Eq. (S.19), where $l_0$ is set to be $l_0 = k_F^{-1}$ (a) and $2k_F^{-1}$ (b). (c) SDOS, $N(E)$, for the bulk s-wave state without surface Dirac fermions, $\text{sgn}(m_0m_1) = +1$, where we set $l_0 = 2k_F^{-1}$.

never mixes, in contrast to the case of the non-topological s-wave pairing. As shown in Figs. S7(b) and S7(c), the resultant energy dispersions are qualitatively same as previous results obtained with a spatially uniform pair potential.4,5,7,8

S6. Tight-binding Hamiltonian and Fermi surface evolution

To clarify the effect of the Fermi surface evolution from the spheroidal to cylindrical shape, we introduce the tight-binding model for superconducting topological insulators. We consider a hexagonal lattice whose primitive vectors are $(\sqrt{3}a/2, a/2, 0)$, $(0, a, 0)$, and $(0, 0, c)$. The tight-binding Hamiltonian is obtained from Eq. (S.15) by replacing $k$

FIG. S7: (a) Spatial profiles of the pair potentials in the topological odd-parity state, the $A_{1u}$ state. The pair potential $\Delta_{\text{bulk}}$ is determined by the amplitude at the center of the system, $\Delta_{\text{bulk}} \equiv \Delta(z = L/2)$. The corresponding energy spectra of quasiparticles at $\tilde{m}_2 = -0.066$ ($\delta = 0.159$) and $-0.20$ ($\delta = 0.08$) are shown in (b) and (c), respectively.
FIG. S8: (a) Shape of the Fermi surface: the spheroidal (the blue curve) and cylindrical (red) Fermi surfaces are given by changing the set of the parameters ($c_1, m_1, v_z$). SDOS’s in the $A_{1u}$ state with the spheroidal Fermi surface (b) and cylindrical Fermi surface (c).

as follows [2]:

$$k_x \rightarrow \frac{2}{\sqrt{3}a} \sin \frac{\sqrt{3}k_x a}{2} \cos \frac{k_y a}{2}, \quad k_y \rightarrow \frac{2}{3a} \left( \cos \frac{\sqrt{3}k_x a}{2} \sin \frac{k_y a}{2} + \sin k_y a \right),$$  \hfill (S.20)

$$k_x^2 + k_y^2 \rightarrow \frac{4}{3a^2} \left( 3 - 2 \cos \frac{\sqrt{3}k_x a}{2} \cos \frac{k_y a}{2} - \cos k_y a \right),$$  \hfill (S.21)

$$k_z \rightarrow \frac{1}{c} \sin k_z c, \quad k_z^2 \rightarrow \frac{2}{c^2} (1 - \cos k_z c),$$  \hfill (S.22)

where $a$ and $c$ are the lattice constants and for Bi$_2$Se$_3$, $a = 4.14\,\text{Å}$ and $c = 28.7\,\text{Å}$. Using the tight-binding Hamiltonian, we self-consistently solve the BdG and gap equations in the $A_{1u}$ state which is the topological odd-parity pairing.

In Fig. S8(a), we show the shape of the Fermi surface in the normal state. For the calculation of the SDOS presented in the main text, we set the parameters as follows: $m_0 = -0.28$ eV, $\mu = 1.8|m_0|$, $c_2 = 30.4$ eVÅ, $m_2 = 44.5$ eVÅ$^2$, and $v = 3.33eV\text{Å}$ as given in Ref. [9]. To change the shape of the Fermi surface, we choose $c_1/c^2 = 0.024$ eV, $m_1/c^2 = 0.20$ eV, and $v_z/c = 0.32$ eV for the spheroidal Fermi surface [2], and $c_1/c^2 = 0.01$ eV, $m_1/c^2 = 0.05$ eV, and $v_z/c = 0.05$ eV for the cylindrical shape. The corresponding SDOS profile for the spheroidal Fermi surface is displayed in Fig. S8(b). Here, the double low-energy peaks are observed, because these values of the parameters indicate that the surface Majorana cone is not twisted [4]. For the spheroidal Fermi surface, as shown in Fig. S8(c), the surface state in the $A_{1u}$ state vanishes, resulting in the simple U-shaped LDOS on the surface.

[1] L. Fu and E. Berg, Phys. Rev. Lett. 105, 097001 (2010).
[2] T. Hashimoto, K. Yada, A. Yamakage, M. Sato, and Y. Tanaka, J. Phys. Soc. Jpn. 82, 044704 (2013).
[3] C.-X. Liu, X.-L. Qi, H.-J. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B 82, 045122 (2010).
[4] A. Yamakage, K. Yada, M. Sato, Y. Tanaka, Phys. Rev. B 85, 180509(R) (2012).
[5] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando, Phys. Rev. Lett. 107, 217001 (2011).
[6] L. A. Wray, S.-Y. Xu, Y. Xia, Y. S. Hor, D. Qian, A. V. Fedorov, H. Lin, A. Bansil, R. J. Cava, and M. Z. Hasan, Nat. Phys. 6, 855 (2010).
[7] T. H. Hsieh and L. Fu, Phys. Rev. Lett. 108, 107005 (2012).
[8] L. Hao and T. K. Lee, Phys. Rev. B 83, 134516 (2011).
[9] C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B 82, 045122 (2010)