Anomalous Josephson current in superconducting topological insulator

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We study the Josephson effect in superconducting topological insulator (STI) by referring to the pairing states of Cu-doped Bi2Se3. The current-phase relation of a junction between even-parity superconductors and STI shows the robust vanishment of the first order component, \( J(\varphi) \sim \sin(2\varphi) \), due to the mirror symmetry of the system. Furthermore, we clarify that the temperature dependence of critical current in junctions consisting of two STIs changes qualitatively depending on the relative spin-helicity of the two surface Andreev bound states. Detecting of these features qualifies as a distinct experimental evidence for the Majorana nature of the Andreev bound states.

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Introduction—Topological superconductors, which support Majorana fermions as gapless Andreev bound states (ABS) on the surface or edge [1–6], are a current hot topic in condensed matter physics. Recently, a new superconductor, Cu-doped Bi2Se3, dubbed as superconducting topological insulator (STI) has been discovered [7, 8]. The presence of zero bias conductance peak in tunneling spectroscopy supports the realization of topological superconducting state in this material [9, 10]. The parent material Bi2Se3 is a topological insulator, which is a band insulator with massless Dirac fermions on the surface [2, 11, 12]. Correspondingly, the STI supports surface Dirac fermions in the normal state. The Dirac fermions can be hybridized with ABSs in the superconducting state, and as a result, the energy dispersion of Majorana fermions in the STI can be different from those in other topological superconductors [13–15]. The difference in the energy dispersion enhances the surface density of state (SDOS) at the Fermi energy, which affects on the tunneling conductance through the surface, remarkably [14–15]. Moreover, several proximity effects [16–18] and Josephson effect [19, 20] of topological insulators have been reported.

The purpose of this letter is to clarify Josephson effect of STI. Josephson effect is one of the most important quantum transport through surfaces in superconductivity. Usually, they are proportional to \( \sin \varphi \), where \( \varphi \) is the phase difference of pair potentials between two superconductors forming the junction. It is well known that \( \pi \)-phase shift [21] has been used for interferometers of Josephson junctions [22, 23], which has established \( d \)-wave symmetry of cuprates [32, 34]. In some \( d \)-wave superconductor junctions, the second-order component of the Josephson effect, \( \sin 2\varphi \), can be dominant in the current-phase relation [35–38]. Furthermore, Josephson junctions between spin-triplet superconductors and spin-singlet ones may show the second order behaviors as well [39–42]. The \( \sin 2\varphi \) behavior, which implies a double degenerate ground state of the junction, is of particular interest since it can be used for a quiet qubit of quantum computers [43]. In the cases mentioned above, however, the second order behavior is easily lost due to the spin-orbit scattering at the interface.

In this letter, we reveal that Josephson effect in STI are characterized by robust second order behaviors in the current phase relation. Based on the symmetry of the system, we first argue that the first-order component \( \sin \varphi \) vanishes even in the presence of the spin-orbit scattering at the interface. Thus the leading term should be the second order. Then, we microscopically calculate the Josephson current for various junctions consisting of STI. For high \( T_c \) cuprates, several interesting features of Josephson current have been found [31, 36–38, 44] due to ABSs [45–47] generated at the interface (surface). For STI, however, there has been no microscopic calculation of Josephson effect up to now. From the microscopic calculation, we establish the second order behavior of the current-phase relation, and clarify that the surface ABS enhances the Josephson current. Furthermore, we find an anomalous behavior of the Josephson current specific to helical Majorana fermions in STI. In particular, it is shown that the magnitude of Josephson current between two STIs is suppressed at low temperature when the spin-helicities of the helical Majorana fermions on the junction are mismatched. The anomalous temperature dependence would provide a unique signal of surface helical Majorana fermions in STI.

Symmetry-based argument—Let us start with a general argument based on symmetry of the system. Josephson current is generally decomposed into a series of different order,

\[
J(\varphi) = \sum_{n=1}^{\infty} (J_n \sin n\varphi + J_n \cos n\varphi).
\]

Under the time-reversal, \( J(\varphi) \) goes to \(-J(-\varphi)\), thus in time-reversal symmetric junctions, \( J(\varphi) \) satisfies

\[
J(\varphi) = -J(-\varphi).
\]

This implies that \( J_n = 0 \) and the leading term is \( J(\varphi) \sim \sin \varphi \).
Now consider symmetry specific to STI. According to Ref. [8], there are four possible gap functions for STI. Among them, however, only the two gap functions that belong to the $A_{1u}$ and $E_u$ representations in the $D_{3d}$ point group are consistent with the tunneling conductance experiment [4, 13]. They both are invariant under time-reversal and they are odd under the inversion, which are responsible for topological superconductivity [8, 5, 6]. They are also odd under the mirror reflection with respect to the $yz$-plane, $(x, y, z) \to (-x, y, z)$. From the mirror symmetry, a structural transition in the energy dispersion of Majorana fermions may occur, which enables us to explain the zero-bias peak of the tunneling conductance observed experimentally [13].

We argue here that the mirror symmetry gives an additional constraint for $J(\varphi)$ [48]. Consider a junction consisting of an $s$-wave superconductor and STI ($s$/STI). The interface of the junction is prepared so as the mirror plane of STI is perpendicular to it. Under the mirror reflection, the STI changes the sign of the gap function, while the $s$-wave superconductor does not. Consequently, one obtains the additional phase of $\pi$ in the Josephson current, $J(\varphi + \pi)$, under the mirror reflection. Therefore the mirror symmetry implies

$$J(\varphi) = J(\varphi + \pi).$$

(3)

This equation yields that $J_{2n+1} = J_{2n} = 0$ in Eq. (1), and the first order term $J(\varphi) \sim \sin \varphi$ vanishes. Thus the leading term is the second order $J(\varphi) \sim \sin 2\varphi$ in the $s$/STI junction. The $\pi$-periodicity of the Josephson current in Eq. (3) is consistent with the effective Josephson coupling $\propto [\Delta_s^2 + \Delta_{s1}^2 + h.c]$ between an $s$-wave gap $\Delta_s$ and the STI one $\Delta_{STI}$ [8].

Our argument above implies that the second order behavior in the $s$/STI junction is robust as far as the time-reversal and the mirror symmetries are preserved. In particular, it is not lost even when the spin-orbit scattering is present in the junction. This is different from previously known second order behaviors in Josephson current. For example, as is the case with STI, a chiral $p$-wave superconductor Sr$_2$RuO$_4$ is a topological superconductor with chiral Majorana edge states [10, 50], and the current phase relation between an $s$-wave and the chiral $p$-wave superconductor is proportional to $\sin 2\varphi$, in the absence of spin-orbit interaction [51, 52]. However, the chiral $p$-wave superconductor is not odd under the mirror reflection, and also breaks the time-reversal invariance. Therefore, the second order behavior is fragile and actually the first-order term $\cos \varphi$ in the current-phase relation appears immediately in the presence of spin-orbit interaction [52].

In the following, we also consider junctions consisting of $d$-wave superconductors and STI. As far as the interface is prepared so as the $d$-wave superconductor is even under the mirror reflection, we have a robust second order behavior of the Josephson current in a similar manner.

**Microscopic calculation**—In the following we calculate Josephson current in STI microscopically. As regards the pairing symmetry of STI, we focus on the $A_{1u}$ representation which is a full-gap topological superconductor, while qualitatively similar results are obtained for the nodal topological superconductor in the $E_u$ representation. As mentioned above, the system has a diagonal mirror plane $(x, y, z) \to (-x, y, z)$, and the gap function is odd under the mirror reflection. We consider various junctions, which consist of (a) $s$-wave superconductor, normal metal (N), and STI $(s$/STI), (b) $d_{x^2-y^2}$-wave superconductor, N, and STI $(d_{yz}$/STI), (c) $d_{xy}$-$d_{x^2-y^2}$-wave superconductor, N, and STI $(d_{yz}$/STI), and (d) STI, N and STI (STI/STI), respectively. The orientation of the superconductors in the junctions are chosen as illustrated in Figs. 1 and 5.

The calculation is based on the three-dimensional square lattice model. We put $s$, $d_{xz}$, $d_{yz}$-$d_{x^2-y^2}$-wave superconductor, or STI in the left region $(1 < z < N_L)$, N in the center region $(N_L + 1 < z < N_L + N_C)$, and STI in the right region $(N_L + N_C + 1 < z < N_L + N_C + N_R)$, respectively. The on-site energy $E_{\sigma_{1,2}}$ and the nearest neighbor hopping along the $z$-direction $t_{A_{1u}}$ with $A = s, d, STI$ are given by $\epsilon_{\sigma} = [2t(\cos k_x + \cos k_y) - \mu_d]\tau_z$, $\epsilon_{\sigma} = [2t \cos k_x + 2t \cos k_y - \mu_d]\tau_z$, $\epsilon_{STI} = \{[m_0 + 2m_1 + 4m_2 - 2m_3(\cos k_x + \cos k_y)]\sigma_x + \nu \sigma_y \sin k_x - \nu \sigma_y \sin k_y - \mu_{STI}\}\tau_z$, $t_{s} = t_{d} = t_{s, d} = \{[m_0 + 2m_1 + i \nu \sigma_y \sin k_x - i \nu \sigma_y \sin k_y - \mu_{STI}]/\tau_z\}$, where $\sigma$, $s$, and $\tau$ are the Pauli matrices in the orbital, spin, and Nambu spaces, respectively. In $s$/STI ($d$/STI) junction, the on-site energy $\epsilon_{N}$ and the hopping $t_{s, d}$ in N are chosen to be the same values as those in the $s$($d$)-wave superconductor: $\epsilon_{N} = \epsilon_{s, d}$. The hopping between the $s$($d$)-wave superconductor and N is assumed to be the same as that in the $s$($d$)-wave superconductor. On the other hand, in STI/STI junction, the transfer at the left interface between STI and N is given by $H_{TL} = \sum_{n} c_{n\sigma s}^{\dagger} t_{LR} \tau_z c_{n+1\sigma s} + h.c.$, with $n = N_L$, and at the right interface, the transfer is $H_{TR} = \sum_{n} c_{n\sigma s}^{\dagger} t_{LR} \tau_z c_{n+1\sigma s} + h.c.$, with $n = N_L + N_R$. Pair potentials of $s$ ($\Delta_s$), $d_{yz}$ ($\Delta_{dyz}$), $d_{x^2-y^2}$ ($\Delta_{dxy}$) -wave superconductors, and STI ($\Delta_{STI}$) are given by $\Delta_s = \sum_{n=1}^{N_L} c_n^{\dagger} \Delta_s \tau_z c_n$, $\Delta_{dyz} = \sum_{n=1}^{N_L} c_n^{\dagger} \Delta_{dyz} \tau_z c_n + h.c.$, $\Delta_{dxy} = \sum_{n=1}^{N_L} c_n^{\dagger} (-\Delta_{dxy} \cos k_y) \tau_z c_n + \sum_{n=1}^{N_L} c_n^{\dagger} \Delta_{dxy} \tau_z c_n + h.c.$, and

$$\Delta_{STI} = \sum_{n=N_L+N_C+N_R}^{N_L+N_C+N_R} c_n^{\dagger} \Delta_{STI} \sigma_y s_{z} (\tau_z \cos \varphi - \tau_y \sin \varphi) c_n.$$

(4)

The temperature dependence of the pair potentials is given as that in the weak coupling limit: $\Delta(T) = \Delta \tan h(1.74\sqrt{T_c/T-1})$, with $\Delta$ being the pair poten-
is the thermal average, and $d$ is the number of the unit cells in the superconductors.

Indeed, under an in-plane Zeeman field $H_Z = \sum_n c_n^\dagger \mathbf{h} \cdot \mathbf{s}_n$ with $h_x = 0$, $h_y = h \sin \theta_h$, $h_z = h \cos \theta_h$, Eqs. (2) and (3) change as $J(\varphi, \theta_h) = -J(-\varphi, \theta_h + \pi)$ and $J(\varphi, \theta_h) = J(\varphi + \pi, \theta_h + \pi)$, respectively, with $J(\varphi, \theta_h)$ the Josephson current under the Zeeman field. From them, we have $J(\varphi, \theta_h) = -J(-\varphi + \pi, \theta_h)$ as a constraint. Therefore, as confirmed numerically for $s$/STI junction under a Zeeman field illustrated in Fig. 3(a), the first order component $\cos \varphi$ can appear in the current-phase relation, while $\sin \varphi$ and $\cos 2\varphi$ cannot [Fig. 3(b)].

Now discuss the free energy of Josephson junctions of STI. The free energy $f$ per unit area of the Josephson junction is given by $f(\varphi) = \hbar/(2e) \int_0^{\pi} d\varphi' J(\varphi')$. Therefore, the second order behavior $J(\varphi) \sim \sin 2\varphi$ implies doubly degenerated ground states in the STI junctions. The minima of $f(\varphi)$ are located at $\varphi = \pm \pi/2$. As discussed in the above, by applying the Zeeman field, the de-
generacy can be lifted. Figure 3(c) shows \( \theta_n \)-dependence of \( f(\varphi) \) at \( \varphi = \pm \pi/2 \), where the free energy \( f(\varphi) \) takes local minima. This figure illustrates that one may choose either of the ground states by applying a suitable Zeeman field.

**Spin-helicity dependent Josephson effect**—Finally, we clarify Josephson effect intrinsic to helical Majorana fermions in STI. As mentioned above, the STI supports helical Majorana fermions on its surface. The effective Hamiltonian of the surface helical Majorana fermion on the interface of junctions (the \( xy \) plane) is represented as

\[
H_{\text{surf}}(k_\parallel) = v_{\text{surf}}(k_x s_y - k_y s_x),
\]

near \( k_\parallel = 0 \). From the Hamiltonian, one can obtain the linear dispersion of Majorana cone, \( E_{\text{surf}} = \pm v_{\text{surf}} k_\parallel \) with \( k_\parallel = |k_\parallel| \). The spin and the momentum are locked on the cone so as the Majorana fermions have a definite eigenvalue \( h_s \) of the spin-helicity \( (k_\parallel \times s)/k_\parallel \) in low energy. From eq. (5), the spin-helicity is \( h_s = \text{sgn}(v_{\text{surf}}) \) for the upper (lower) cone. A unique character of Majorana fermions in STI is that the spin-helicity can change depending on the chemical potential \( \mu \). We also find that when \( \mu_{\text{STI}} < \mu_{\text{STI}}^L \), the energy dispersion of the Majorana fermion is not a simple cone, but a rather complicated caldera-shaped one. As a result, in addition to the cone with \( h_s = - \) near \( k_\parallel = 0 \), there is another branch with \( h_s = + \) in the spectrum, as illustrated in Fig. 4. Referring to the spin-helicity of the upper cone near \( k_\parallel = 0 \), we denote STI with a simple cone and that with a complicated caldera-shaped one as STI(+) and STI(−), respectively.

Now let us study the spin-helicity dependence of Josephson current. For this purpose, we consider STI/STI junction illustrated in Fig. 5. By tuning the chemical potentials in the left and right STIs, we can change the spin-helicity of the Majorana cone in each STI. We calculate the Josephson current of STI/STI junctions with three different combinations of spin-helicity, STI(+) STI(+), STI(+) STI(−), and STI(−) STI(−), respectively. In these junctions, the current-phase relation of \( J(\varphi) \) is rather conventional, however, the temperature dependence becomes anomalous. Figure 5 shows the temperature dependence of the maximum Josephson current \( J_{\text{max}}(T) \) for these junctions. We find that, as compared to the junctions with the same spin-helicity, i.e. STI(+) STI(+) and STI(−) STI(−) junctions, the Josephson current with the mismatched spin-helicity [STI(+) STI(−) junction] is strongly suppressed. In particular, we find that the Josephson current of the latter junction decreases at low temperature while those of the former increases. Here we note that the suppression in the mismatched case occurs below \( T/T_{\text{cSTI}} \sim 0.07 \), which exactly corresponds to the energy \( |E/\Delta| < 0.07 \) where the \( h_s = - \) branch appears in STI(−) [See Fig. 3(b)]. This implies that the suppression of the Josephson current occurs due to the mismatch of the spin-helicity in the junction. We also find that the Josephson current in STI(−) STI(−) is much more enhanced at low temperature than that in STI(+) STI(+) because a twisted energy spectrum of the caldera cone has many low-lying states which contribute to Josephson current. We would like to mention here that the spin-helicity dependence of the Josephson current is different from that of two-dimensional helical superconductors since the Josephson current in two-dimensional helical superconductors is always enhanced at low temperature, independent of the spin-helicity.
Discussions—The anomalous Josephson effect reported in this letter are accessible experimentally: First, the vanishment of $\sin \varphi$- and $\cos \varphi$-terms in the current-phase relation in $s$/STI and $d$/STI junctions is detectable by the Shapiro steps at the bias voltage given by $V = n \hbar \omega / (4e)$, where $n$ is an integer and $\omega$ is the frequency of the microwave. The DC-SQUIDs with these junctions are also very sensitive to the second order behavior $\sin 2\varphi$ of the current-phase relation. Moreover, the anomalous temperature dependence of STI/STI junctions is easily measurable in experiments. The anomalous temperature dependence is of particular interest since it is a direct experimental signal of the spin-lock nature of surface helical Majorana fermions, and thus a direct experimental evidence of topological superconductivity of STI.

To summarize, we have shown that Josephson current between even-parity superconductors and STI can be robustly proportional to $\sin 2\varphi$ as far as the mirror symmetry of the system is preserved. Therefore, Cu$_2$Bi$_2$Se$_3$ is a good platform to realize a Josephson junction with $\sin 2\varphi$-current-phase relation and two-fold degenerated ground states, which can be utilized for quiet qubit in quantum computing. We have also clarified that the magnitude of the Josephson current in STI/STI junction is influenced critically by the relative spin-helicity between the surface helical Majorana fermions of the two STIs. Although the existence of surface gapless states has been experimentally confirmed in Cu$_2$Bi$_2$Se$_3$ by tunneling spectroscopy [3], which is consistent with topological superconductivity in Cu$_2$Bi$_2$Se$_3$ [14, 15, 55], their Majorana nature has not yet. The spin-helicity dependent Josephson current could be an experimental signal that is directly related to the Majorana fermions on the surface of STI.

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