Quantum thermal Hall effect of Majorana fermions on the surface of superconducting topological insulators

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We study the quantum anomalous thermal Hall effect in a topological superconductor which possesses an integer bulk topological number, and supports Majorana excitations on the surface. To realize the quantum thermal Hall effect, a finite gap at the surface is induced by applying an external magnetic field or by the proximity effects with magnetic materials or s-wave superconductors with complex pair-potentials. Basing on the lattice model Hamiltonian for superconducting states in Cu-doped Bi$_2$Se$_3$, we compute the thermal Hall conductivity as a function of various parameters such as the chemical potential, the pair-potential, and the spin-orbit coupling induced band gap. It is argued that the bulk topological invariant corresponds to the quantization rule of the thermal Hall conductivity induced by complex s-wave pair-potentials.

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I. INTRODUCTION

Topological insulators and superconductors are new quantum states of matter, characterized by topological numbers. The quantum Hall effect (QHE) is a first found topologically nontrivial state, where the Hall conductivity is quantized as

$$\sigma_{xy} = \nu \frac{e^2}{h},$$

\(\nu\) being an integer value corresponding to the topological number of bulk wave functions. The two-dimensional (2d) topological superconductors and superfluids with chiral (p-wave) Cooper pairing are superconductor analogues of the QHE and considered to be realized, e.g. in a thin film of $^3$He A phase, Sr$_2$RuO$_4$, and the 5/2-filling fractional QHE. In superconductors, charges are not conserved and thus electric transport study such as quantum Hall measurement cannot characterize their topological nature. Instead, since the energy is still conserved, thermal transport especially the thermal Hall conductivity reflects the topological character of topological superconductors as

$$\kappa_{xy} = \nu \frac{\pi^2 k_F^2}{6\hbar T}.$$  

Here \(\nu\) corresponds to the bulk topological number.

Recent studies have shown that topological states exist in time-reversal invariant and three-dimensional (3d) cases as well. The surface of three-dimensional topological insulators supports gapless excitations with a linear dispersion, for some simple cases, which can be described by the two-dimensional massless Dirac Hamiltonian. One of the intriguing phenomena is the quantum anomalous Hall effect on the surface of topological insulators. Recently, the experimental observation of the quantum anomalous Hall effect was reported in Cr-doped (Bi,Sb)$_2$Te$_3$ thin films, where the Hall conductivity exhibits a clear quantized plateau, accompanied by a considerable drop in the longitudinal resistance.

Theoretically the systematic classification of topologically nontrivial insulators and superconductors is established in terms of symmetries and dimensionality, and clarified that topologically nontrivial superconductors (TSCs) and superfluids (TSFs) with time-reversal symmetry are also realized in three-dimensions. In contrast to three-dimensional topological insulators which are characterized by \(\mathbb{Z}_2\) topological numbers, three-dimensional topological superconductors are characterized by integers \(\mathbb{Z}\). An example of 3d-TSCs is the B phase of superfluid $^3$He. From the bulk-boundary correspondence, there exist topologically protected gapless Andreev bound states in TSCs. In particular, the superconductivity infers that the gapless Andreev bound states are their own antiparticles, thus Majorana fermions.

On the surface of $^3$He B phase, a clear linear dispersion of in-gap states was measured experimentally. In addition, the newly found superconducting phase in Cu-doped Bi$_2$Se$_3$ has been proposed to be a 3d-TSC. Recently, point-contact spectroscopy experiments in Cu-doped Bi$_2$Se$_3$ have reported a zero-bias conduction peak which is in debate whether it indicates gapless surface modes with characteristic dispersion relations modified from the linear Majorana cone or not.

As surface Dirac fermions realize the anomalous quantum Hall effect in topological insulators, the anomalous quantum thermal Hall effect of Majorana fermions occurs on the surface of topological superconductors. For the ideal case where surface spectra have a linear Dirac-Majorana dispersion such as $^3$He B phase, the thermal Hall conductivity can be easily evaluated as

$$\kappa_{xy} = \pm \frac{\pi^2 k_F^2}{2\hbar T}.$$  

On the other hand, it is not obvious what the value of the thermal Hall conductivity is in the case of Cu-doped Bi$_2$Se$_3$ with modified surface dispersions. In addition, it would be natural to question whether the quantized thermal Hall conductivity is related to the bulk topological number.

In this work we study anomalous thermal transport on the surface of superconducting doped topological insu-
We first calculate the phase diagram of the effective Bogoliubov-de Genne Hamiltonian for the bulk case, as a function of the original band gap of the host material, the chemical potential, and the superconducting pair-potential. There exist different types of gapped superconducting states. We characterize the gapped states by computing the topological numbers in the bulk and the thermal Hall conductivity in a slab geometry.

The phase transitions are signaled by the vanishing excitation gap in Fig. 4. In the normal case, $\Delta = 0$, the excitation gap is finite only when the chemical potential is in the original band gap, $|\mu| \leq M_0$ (phase I). When the chemical potential is above the band gap, $|\mu| > M_0$, the system is in the metallic phase. The finite excitation gap is induced by the nonzero pair-potential $\Delta$. Within the parameter region of Fig. 4 there are two superconducting phases, phase II and phase III, distinguished by gap vanishing. In the following, we will see that one of the superconducting state (phase II) is topologically nontrivial while the other (phase III) is trivial. In phase I, since the chemical potential $\mu$ is located

\[ R_1(k) = A_1 \frac{2}{\sqrt{3}} \sin \left( \frac{\sqrt{3}}{2} k_y a \right) \cos \left( \frac{1}{2} k_y a \right) \]

\[ R_2(k) = A_2 \frac{2}{\sqrt{3}} \left( \cos \left( \frac{\sqrt{3}}{2} k_y a \right) \sin \left( \frac{1}{2} k_y a \right) + \sin \left( k_y a \right) \right) \]

\[ R_3(k) = A_3 \sin (k_y c) \]

\[ M(k) = M_0 - B_1 \left[ 2 - 2 \cos (k_y c) \right] - \frac{4}{3} B_2 \left[ 3 - \cos (k_y a) \right] - 2 \cos \left( \frac{\sqrt{3}}{2} k_y a \right) \cos \left( \frac{1}{2} k_y a \right) \]

\[ \epsilon(k) = -\mu + D_1 \left[ 2 - 2 \cos (k_y c) \right] + \frac{4}{3} D_2 \left[ 3 - \cos (k_y a) \right] - 2 \cos \left( \frac{\sqrt{3}}{2} k_y a \right) \cos \left( \frac{1}{2} k_y a \right) \].
in the original band gap, and thus the density of states vanishes, it is hardly expected that the superconducting order is developed spontaneously. In this sense, phase I is an artifact introduced by assuming a finite bulk pair-potential. Nevertheless it is of theoretical interest to see how two Majorana dispersions contribute to the thermal Hall conductivity as discussed in VI. Figure 2 shows the excitation gap as a function of the chemical potential $\mu$ and the band gap parameter $M_0$, where the pair-potential is fixed at $\Delta = 0.05$ [eV]. This result indicates that beside the topological insulating state (phase I), there are three superconducting gapped states (phase II, III, and IV) which are separated by gap closing.

IV. SYMMETRIES AND TOPOLOGICAL NUMBERS

Here we study the topological properties of the phases appeared in the phase diagram by computing the topological numbers. The Bogoliubov-de Genne Hamiltonian has both time-reversal ($\Theta$) and particle-hole ($\Xi$) symmetries,

$$\Theta^{-1} \mathcal{H}_{BdG}(k) \Theta = \mathcal{H}_{BdG}(-k)$$  
(9)

$$\Xi^{-1} \mathcal{H}_{BdG}(k) \Xi = -\mathcal{H}_{BdG}(-k).$$  
(10)

Because of these symmetries, one can find a unitary matrix $\Gamma = \Theta \Xi$ that anticommutes with the Hamiltonian

$$\Gamma^{-1} \mathcal{H}_{BdG}(k) \Gamma = -\mathcal{H}_{BdG}(k).$$  
(11)

This chiral symmetry implies that eigenenergies of the Bogoliubov-de Genne Hamiltonian (eq. (4)) appear as pairs of $\pm E_n(k)$:

$$\mathcal{H}_{BdG}(k) \left| u^+_n(k) \right> = \pm E_n(k) \left| u^+_n(k) \right>$$  
(12)

Here we introduce the $Q$-matrix defined as

$$Q(k) = \sum_n \left( \left| u^+_n(k) \right> \left< u^+_n(k) \right| - \left| u^-_n(k) \right> \left< u^-_n(k) \right| \right).$$  
(13)

FIG. 3. Winding number defined by eq. (15) is plotted as a function of the original band gap $M_0$. The chemical potential is fixed at (a) $\nu = 0.6$ [eV] (a) and (b) $\nu = 0.2$ [eV].
As a consequence of chiral symmetry eq. (11), the $Q$ matrix can be brought into block off-diagonal form,

$$Q(k) = \begin{bmatrix} 0 & q(k) \\ q^T(k) & 0 \end{bmatrix}, \quad q(k) \in U(4) \tag{14}$$

in the basis in which $\Gamma$ is diagonal. The topological index in the presence of chiral symmetry is given by the winding number $\nu$:

$$\nu = \int \frac{d^3k}{24\pi^2} \epsilon_{\mu\nu\rho} \text{tr} \left[ (q^{-1} \partial_\rho q)(q^{-1} \partial_\rho q)(q^{-1} \partial_\rho q) \right] \tag{15}$$

which takes integer values, where $\mu, \nu, \rho = k_x, k_y, k_z$, and the integral extends over the entire Brillouin zone. As shown in Fig. 3, the evaluated values of $\nu$ are 0, 1, 0, and -1 in phase I, II, III, and IV, respectively.

V. SURFACE MODES OF TOPOLOGICAL SUPERCONDUCTORS

To study the energy dispersion of surface modes, and compute the thermal Hall conductivity, we consider a slab geometry of topological superconductors. The normal part of the Hamiltonian can be written as

$$H_0 = \sum_{k_{\perp}, j} \left[ c_{k_{\perp}, j}^\dagger (\hat{h}_{k_{\perp}}) c_{k_{\perp}, j} + c_{k_{\perp}, j+1}^\dagger h_z c_{k_{\perp}, j} \right] + \epsilon'(k_{\perp}) I \tag{16}$$

where $k_{\perp} = (k_x, k_y)$, $j$ is the position in $z$ direction: $j = L_z$ and $j = 1$ correspond to the top and bottom surfaces, respectively. In eq. (16), we omit the band and spin indices. In eq. (17),

$$h_{\perp}(k_{\perp}) = \sum_{a=1, 2} R_a(k_{\perp}) \alpha_a + M'(k_{\perp}) \beta + \epsilon'(k_{\perp}) I \tag{17}$$

and

$$h_z = \frac{i}{2} A_3 \alpha_3 + B_1 \beta - D_1 I \tag{18}$$

describe spin-dependent hopping in $x$-$y$ plane and in $z$ direction, respectively, where

$$M'(k) = M_0 - 2B_1 - \frac{4}{3} B_2 \left[ 3 - \cos(k_y a) \right]$$

$$-2 \cos \left( \frac{\sqrt{3}}{2} k_x a \right) \cos \left( \frac{1}{2} k_y a \right) \tag{19}$$

$$\epsilon'(k) = -\mu + 2D_1 + \frac{4}{3} D_2 \left[ 3 - \cos(k_y a) \right]$$

$$-2 \cos \left( \frac{\sqrt{3}}{2} k_x a \right) \cos \left( \frac{1}{2} k_y a \right). \tag{20}$$

The pair-potential part, $\Delta$, is independent of both the momentum and the position. We obtain the matrix element of the total Hamiltonian in the basis of $\{|k_{\perp}, j\rangle\}$. By diagonalizing the Hamiltonian matrix, eigenenergies $E_{n, k_{\perp}}$ and eigenstates $|n, k_{\perp}\rangle$ are obtained.

Typical results of the spectrum are shown in Fig. 4 for (a) phase II, (b) phase IV, (c) phase I, (d) phase III as labeled in Fig. 3. The presence/absence of the surface modes indicates that these are topological/trivial superconducting states. In Fig. 3 (a) simple Majorana cone is seen as expected from previous work. As the chemical potential closes to the bottom of the conduction band, the surface spectrum deform from the simple Majorana cone as discussed in Refs. [24] and [25]. Such deformed surface Majorana mode can be seen also in phase IV (Fig. 4 (b)). In phase I Majorana modes are doubled. This can be understood as follows. In the normal limit, $\Delta = 0$, phase I is a topological insulating state which has a single Dirac cone on the surface. As a pair-potential $\Delta$ is induced, the complex fermions are split into two independent Majorana modes. A similar situation has been discussed in a quantum anomalous Hall insulator/spin-singlet $s$-wave superconductor hybrid system [26]. In the next section, we discuss the connection between these surface modes and the quantized thermal Hall conductivity.

VI. ANOMALOUS THERMAL HALL CONDUCTIVITY

When the surface modes have a finite gap, the quantum thermal Hall effect occurs. Physically the gap is induced by the magnetic interactions. Figure 6 (a) depicts an experimental setup where the interactions between quasiparticles and magnetizations in ferromagnets (or magnetic dopants such as Cr as in Ref. [13]) near the surface are introduced. A similar situation is realized by
applying an external magnetic field. Due to the Meissner effect, the field can be finite within the penetration depth from the surface. The magnetic interaction term is given by

$$H_{\text{exc}} = \sum_{\mathbf{k}_{\perp}, \mathbf{j}} \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}}^\dagger J M_z(j) \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}},$$  

(21)

where $J$ is the exchange interaction constant and $M_z$ is the mean value of magnetic moments. For simplicity, we consider the case where magnetic moments are finite only at the top ($j = 1$) and bottom ($j = L_z$) surfaces, while zero in the bulk.

To compute the thermal Hall conductivity, we use the generalized Wiedemann-Franz law \cite{38-40} to the case of Majorana fermions \cite{38-40}.

$$\kappa_{xy} = \frac{\pi^2 k_B^2 T}{6L^2} \sum_{n,m} \sum_{\mathbf{k}_{\perp}} \theta(-E_n\mathbf{k}_{\perp}) \frac{2 \text{Im}[\langle n, \mathbf{k}_{\perp}|\mathbf{v}_n|n, \mathbf{k}_{\perp}\rangle \langle m, \mathbf{k}_{\perp}|\mathbf{v}_n|m, \mathbf{k}_{\perp}\rangle]}{(E_n\mathbf{k}_{\perp} - E_m\mathbf{k}_{\perp})^2}.$$  

(22)

where $L^2$ is the area of the surface. Apart from the factor $\pi^2 k_B^2 T/6$, the right hand side resembles the Kubo formula for the electrical Hall conductivity, which, however, is not a well-defined quantity for Majorana fermions; nevertheless Eq. (22) can be regarded as the generalized Wiedemann-Franz law to Majorana fermions. Compared to the electron systems, there is an extra factor of 1/2 due to Majorana nature.

The thermal Hall conductivity $\kappa_{xy}$ is shown in Fig. 5 as a function of the chemical potential $\mu$. Quantized values in units of $\pi^2 k_B^2 T/6h$ are clearly seen. Figure 5 (b) and (c) show $\kappa_{xy}$ in the presence of the magnetic interaction (Fig. 5 (a)). At the chemical potential $\mu = 0.6$ [eV], the thermal Hall conductivity changes from $1 \rightarrow 0 \rightarrow 1$ as shown in Fig. 5 (b) while the phase changes as II $\rightarrow$ III $\rightarrow$ IV. At $\mu = 0.2$ [eV] (c), $\kappa_{xy}$ changes $1 \rightarrow 2 \rightarrow 1$, while the phase changes as II $\rightarrow$ I $\rightarrow$ IV. These results show that the quantized thermal Hall conductivity induced by the magnetic interaction can distinguish phase I and III. Moreover the quantized values characterize the number of surface Majorana dispersions. The result $\kappa_{xy} = 2 \times \pi^2 k_F^2 T$ in phase I is consistent to the fact that the surface modes in phase I are two split Majorana modes as shown in Fig. 5 (c). Similarly, $\kappa_{xy} = 0$ is consistent to the absence of surface modes in phase III, indicating that this phase is topologically trivial.

The other way to open a gap in the surface spectrum is introducing $s$-wave pairing with an imaginary pair-potential on the surface by the proximity effect with ordinary superconductors (SC) as proposed in Ref. \cite{27} (Fig. 5 (d)). In our model Hamiltonian, this interaction is described by

$$H_{\text{SC}} = \sum_{\mathbf{k}_{\perp}, \mathbf{j}} \left[ \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}}^\dagger \Delta_s(j) \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix} \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}}^T + \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}}^\dagger \Delta_s(j) \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix} \varepsilon_{\mathbf{k}_{\perp}, \mathbf{j}} \right].$$  

(23)

Because of the proximity effect, we assume that $\Delta_s$ is finite only at the top and bottom surfaces. When the $s$-wave pair-potentials, $\Delta_s$, have opposite sign between top and bottom, $\kappa_{xy}$ becomes finite. Figures 5 (e) and (f) both show that $\kappa_{xy}$ changes as $1 \rightarrow 0 \rightarrow -1$. At the chemical potential $\mu = 0.6$ (e), the phase changes as II $\rightarrow$ III $\rightarrow$ IV. On the other hand, at the chemical potential $\mu = 0.2$ (f), the phase changes as II $\rightarrow$ I $\rightarrow$ IV. The results shown in Fig. 5 (e) and (f) indicate that $\kappa_{xy}$ vanishes in phase I and III. The quantum thermal Hall effect induced by $s$-wave pair-potential does not distinguish the topological nature of phase I and III.

Let us compare the thermal Hall conductivity obtained above and the bulk topological number $\nu$. As shown in Fig. 5, $\nu$ changes as $1 \rightarrow 0 \rightarrow -1$ as the phase changes II $\rightarrow$ III $\rightarrow$ IV and also II $\rightarrow$ I $\rightarrow$ IV. These behaviors are identified to the quantization rule of $\kappa_{xy}$ when the TSC is attached to the mirror Chern number, even in topologically trivial phases. Instead of the bulk topological number $\nu$, the integers appeared in $\kappa_{xy}$ could be connected to the mirror Chern numbers. Interestingly, the Mirror Chern number in phase I is $2\mu$ as the energy dispersion of the surface modes, Fig. 5 indicates. This number is consistent to $\kappa_{xy} = 2 \times \pi^2 k_F^2 T$ in phase I. Since no physical observables connected to the mirror Chern number have yet been predicted, it is of great interest if one can show that the thermal conductivity could be related the mirror Chern number under some symmetry conditions. To confirm this statement, further investigation is needed and done elsewhere.

VII. DISCUSSION

Time-reversal invariant topological superconductors in three-dimensions (class DIII) are characterized by integers $\mathbb{Z}$ in contrast to topological insulators (class AII) which have $\mathbb{Z}$ numbers. \cite{41} In this paper we studied the relation between the topological invariant and the thermal Hall conductivity, basing on the model for superconducting states in Cu-doped Bi$_2$Se$_3$. The thermal Hall conductivity shows different behavior when the surface gap is induced by the magnetic interactions and by the complex $s$-wave pair-potentials. As discussed in Ref.
FIG. 5. (Color online) Top: Illustrating the experimental setting for the measurement of the quantum thermal anomalous Hall effect of Majorana fermions on the surface of a three-dimensional topological superconductor with (a) attached ferromagnetic insulators and (d) attached s-wave superconductors with complex pair-potentials. Bottom: Thermal Hall conductivity $\kappa_{xy}$ as a function of the band gap $M_0$ in units of $\pi^2 k_B^2 T/6\hbar$ is plotted in (b), (c), (e), and (f). The case of ferromagnets attached on the top and bottom surfaces is shown in (b) $\mu = 0.6 \text{ [eV]}$ and (c) $\mu = 0.2 \text{ [eV]}$. The bulk pair-potential is fixed at $\Delta = 0.05 \text{ [eV]}$, $\kappa_{xy}$ with s-wave pairing induced by the proximity effect is shown in (e) $\mu = 0.6 \text{ [eV]}$ and (f) $\mu = 0.2 \text{ [eV]}$. 

We confirmed that the topological invariants of time-reversal invariant superconductors in three dimensions are directly related to the surface thermal Hall conductance induced by the complex s-wave pair-potentials.

The quantum thermal Hall effect on the surface of topological superconductors are closely related to the cross-correlated thermal responses of topological superconductors. Since gauge symmetry is spontaneously broken in superconducting phases, it is useful to consider responses to the gravitational fields instead of electromagnetic fields. In Refs. [24] and [27], we confirmed that the gravitational instanton term was introduced to characterize the thermal responses, because the gravitational fields can be connected to the thermal gradients. It was argued that the gravitational instanton term can characterize only the $\mathbb{Z}_2$ part of topological classification.

Later the energy density functional which characterizes the cross-correlated responses between the thermal gradient and mechanical rotational motion with full $\mathbb{Z}$ classification of three-dimensional topological superconductors was derived in Ref. [28]. The strength of these couplings, however, were found to be very small, and thus the effect may not be measurable. The present work concludes that topological invariants of three-dimensional topological superconductors can be measured by thermal transport on the surface subjected to the proximity with complex s-wave pairing field.

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When the width of the system is not large enough, the positions where \( \kappa_{xy} \) changes differ from the phase transition points of the bulk system.

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