Hall conductivity as bulk signature of topological transitions in superconductors

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Abstract – Topological superconductors (TSCs) may undergo transitions between phases with different topological numbers which are related to the presence of gapless (Majorana) edge states. In a TSC the charge Hall conductivity, $\sigma_{xy}$, is not quantized and evolves continuously between different topological phases. Here we show that in two-dimensional Z-TSC the derivatives of $\sigma_{xy}$ display sharp features signaling the topological transitions. We consider in detail the case of a triplet superconductor with $p$-wave symmetry in the presence of Rashba spin-orbit coupling and externally applied Zeeman spin splitting. We generalize to the cases where the normal system is already topologically non-trivial.

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Introduction. – In two dimensions, $\mathbb{Z}$ topological insulators exhibit a charge Hall conductivity, $\sigma_{xy}$, that is quantized and proportional to the Chern number of the occupied bands [1–3]. Such non-trivial topological phases are also characterized by the presence of gapless edge modes [4,5] that can be detected by transport measurements or tunneling. In a topological superconductor (TSC) one does not expect $\sigma_{xy}$ to be quantized, however, as charge is not conserved due to the breaking of $U(1)$ symmetry. In a singlet superconductor (SC) spin is conserved and there is still a possibility that the spin Hall conductivity is quantized, as previously shown for a $d$-wave SC in the vortex state [6]. For a triplet SC even this quantization is absent. The thermal Hall conductivity has recently been shown to be quantized for TSCs with broken time-reversal symmetry (TRS) [7].

Generally speaking, the charge Hall resistance may be written as the sum of two contributions, one proportional to the magnetic field and an anomalous contribution as $\rho_{xy} = R_0 H_z + \rho_{xy}^{\text{AH}}$ (considering $z$ as the perpendicular direction to the plane where the charges move). The term $\rho_{xy}^{\text{AH}}$ is the anomalous Hall effect and has different origins [8]. One of these is intrinsic and stems from a non-zero Berry curvature, leading to an anomalous velocity [9,10]. An anomalous velocity may also be due to scattering mechanisms from impurities in systems where the spin-orbit (SO) is present, such as the skew scattering and the side jump [11,12].

Historically, the anomalous Hall resistivity was studied in detail in systems with a finite magnetization, $M_z$, where $\rho_{xy}^{\text{AH}} = R_s M_z$ [8]. Anomalous properties in SCs with magnetization have been studied, in particular, the presence of muonoclectric effects [13], the generation of a charge Hall effect due to a spin current [14] or a spin Hall effect due to a charge current [15]. The anomalous Hall effect has been studied [16] in SCs with SO coupling. The presence of a magnetic impurity in a conventional SC already induces a non-vanishing $\sigma_{xy}$. In the case of triplet SCs, $\sigma_{xy}$ was also shown to be non-vanishing if SO coupling is present [16].

In this work we will be concerned with the effect of the intrinsic contribution to $\sigma_{xy}$ in Z-TSCs. Superconductivity with non-trivial topology may be obtained in different ways [3]. It can be due to the pairing symmetry, as is the case of $p$-wave SCs [17]. In semiconductors with Rashba SO coupling it arises when $s$-wave superconductivity is induced and a Zeeman term is added [18,19]. An interesting proposal is that of systems where the normal phase is already topologically non-trivial, in which case a TSC can be obtained if $s$-wave superconductivity is induced by the proximity effect [20,21]. Here we consider a Rashba-type non-centrosymmetric SC with admixture of $s$-wave and $p$-wave pairing and TRS breaking Zeeman splitting, which has been recently proposed in ref. [22].

As the Hamiltonian parameters change, different topological phases appear. Their appearance and transitions have been proposed to be detected in various ways, such as
the detection of the Majorana end states in zero-bias peaks in tunneling spectroscopy experiments [23–26], including spatially resolved peaks [27], anomalous Fraunhofer patterns and fractional Josephson effects [28–30]. Multiple Andreev reflection current in voltage-biased junctions has also been proposed as a signature of topological order [31] in particular in the derivative of the current and in the zero-bias conductance of nodal non-centrosymmetric SCs [32]. The imaginary part of $\sigma_{xy}$ at finite frequency may also be used to signal topological phases [33].

The main results of this paper may be summarized as follows. Whenever a $Z$-TSC is realized we find that the behavior of $\sigma_{xy}$ and its derivatives with respect to the parameters that drive the topological transition, specially the second derivative, provide an alternative way to signal topological transitions in SCs. Across a topological transition $\sigma_{xy}$ is rather smooth, in contrast to the sharper change in the case of the non-topological transition induced by a magnetic impurity [16]. We note that even though the thermal Hall conductivity is quantized and provides a direct characterization of a topological phase, though the thermal Hall conductivity is quantized and allowed [38]. Therefore, we also consider a contribution from $s$-wave pairing [16,22]. We write the Hamiltonian as

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}} \left( c_{k}^{\dagger} c_{-k} + \Delta_{0}(\mathbf{k}) \right) \left( \hat{\Delta}(\mathbf{k}) - \hat{\Delta}^{\dagger}(\mathbf{k}) \right) \left( c_{k}^{\dagger} c_{-k} \right),$$

where $(c_{k}^{\dagger} c_{-k}) = (c_{k_{1}^{\uparrow}}^{\dagger} c_{-k_{1}^{\downarrow}}, c_{-k_{1}^{\uparrow}} c_{k_{1}^{\downarrow}})$ and $\Delta_{0} = \epsilon_{k} \sigma_{0} - M_{z} \sigma_{z} + H_{R}$. Here $\epsilon_{k} = -2t(\cos k_{x} + \cos k_{y}) - \epsilon_{F}$, where $t$ is the hopping parameter, $\epsilon_{F}$ the chemical potential, and $M_{z}$ is the Zeeman splitting term. We use units such that $\hbar = 1$, where $a$ is the lattice constant. The Rashba SO term is written as $H_{R} = s \cdot \sigma = \sigma_{x} (\sin k_{y} - \sin k_{x})\sigma_{y}$, where $s = \alpha(\sin k_{y} - \sin k_{x}, 0)$. The matrices $\sigma_{x}, \sigma_{y}, \sigma_{z}$ are the Pauli matrices acting on the spin sector, and $\sigma_{0}$ is the $2 \times 2$ identity.

The pairing matrix reads $\Delta = i(\mathbf{d} \cdot \mathbf{\sigma} + \Delta_{0}) \sigma_{y}$. The vector $\mathbf{d} = (d_{x}, d_{y}, d_{z})$ is the vector representation of the $p$-wave superconducting pairing and is an odd function of $\mathbf{k}$. Because of Fermi statistics, the pairing matrix satisfies $\Delta(k) = -\Delta^{\dagger}(-k)$. The triplet pairing term is invariant under a spin rotation about the $\mathbf{d}$-direction. We note that both superconductivity and magnetization $M_{z}$ may be due to intrinsic order or to some proximity effect. The pairing matrix for a $p$-wave SC generally satisfies $\Delta \Delta^{\dagger} = |\mathbf{d}|^{2} \sigma_{0} + \mathbf{q} \cdot \mathbf{\sigma}$, where $\mathbf{q} = \mathbf{i} \mathbf{d} \cdot \mathbf{d}^{\ast}$. If the vector $\mathbf{q}$ vanishes the pairing is called unitary ($s$-wave pairing is always unitary). Otherwise, it is called non-unitary [39], breaks TRS and originates a spontaneous magnetization, as in $^{3}$He We will consider both unitary and non-unitary pairings.

In the case of unitary pairing we consider two regimes. One where the pairing is aligned [40] along the SO vector $\mathbf{s}$. This is expected if the SO is strong since it is energetically favorable, and we refer to it as the strong SO regime. In the other, called weak SO regime, we will allow the two vectors to be misaligned.
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Chern numbers and Hall conductivity.

Weak SO coupling. Figure 1 shows $\sigma_{xy}$ as calculated from the Kubo formula given in eq. (10) of ref. [16]. We consider the unitary and the non-unitary cases, relaxing the restriction that $d \parallel s$ which was assumed in ref. [22]. The two cases are chosen as $d_x = d \sin k_y, d_y = d \sin k_x, d_z = 0$ and $d_x = -d/2 \sin k_x = -i d_y, d_z = 0$, respectively. The behavior of $\sigma_{xy}$ in the unitary phase is similar to that in a normal system (not shown). Both require $M_z \neq 0$ to obtain a non-zero $\sigma_{xy}$. In the non-unitary case, the vector $q$ induces a magnetization that already produces a finite $\sigma_{xy}$ even if $M_z = 0$. In all cases the SO coupling is necessary for a finite $\sigma_{xy}$ to show up.

In all three cases (normal, unitary, and non-unitary), $\sigma_{xy}$ has a clear minimum when the magnetization is of the order of the chemical potential. At this point the spectrum is gapless and the Chern number of the occupied bands changes. The topological transition does not depend on $\alpha$ and the $C$ evolution is shown in fig. 1 for $\alpha = 1$ in the unitary case. It turns out that for the non-unitary case the spectrum is always gapless since the pairing function does not depend on $k_y$. Considering a non-unitary pairing of the form $d_x = d \sin k_y, d_y = i d \sin k_x, d_z = 0$ the behavior of $\sigma_{xy}$ and $C$ is similar to that obtained in fig. 1 for the unitary case. In the normal phase the system is topologically trivial with $C = 0$ throughout the space of parameters.

Strong SO coupling. For strong SO coupling it has been shown that the alignment of the pairing vector $d$ with the SO vector $s, d = d s/\alpha$ leads to a higher critical temperature [40]. There is a rich sequence of topological transitions as a function of chemical potential, SO coupling, and magnetization [22].

In fig. 2 we show the results for the Chern number of the occupied bands as a function of the chemical potential and magnetization. The result for $\sigma_{xy}$ is also shown in the same parameter region. Even though $\sigma_{xy}$ is a continuous, smooth function there are clearly local maxima and minima that can be associated with topological transitions.

In the case of a $\mathbb{Z}$ topological insulator, a topological transition modifies the Chern number and the quantized

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1 In ref. [16] the amplitude $v_n(-k, \uparrow)$ in eq. (2) should have a minus sign. This led to numerical results for $\sigma_{xy}$ that were not correct and are corrected in this manuscript. The conclusions of ref. [16] remain valid as there is no qualitative change of the results.
its first derivative are multiplied by a factor of 10.

The Hall conductivity and value of \( \sigma \) vs. magnetization or chemical potential for strong SO coupling. The Hall conductivity and its first derivative are multiplied by a factor of 10.

value of \( \sigma_{xy} \), which, therefore, exhibits a clear signature of the transition. In the case of a \( Z \)-TSC there is no discontinuity in \( \sigma_{xy} \). However, its second derivative signals the transitions sharply. This is well illustrated in fig. 3 where we show cuts at constant chemical potential as a function of \( M_z \) and \( \epsilon_F \). The results for the Chern number clearly indicate the topological transitions either as a function of \( M_z \) or \( \epsilon_F \). The behavior of \( \sigma_{xy} \) correlates with these transitions. As expected from general considerations, if a transition occurs between Chern numbers of different signs, \( \sigma_{xy} \) changes sign accordingly. Here we are interested in finding a signature of the change in the Chern number. This can be achieved by looking at the derivatives of \( \sigma_{xy} \). At the transitions the derivative behaves in a way qualitatively similar to the case of a \( Z \) topological insulator: if the Chern number increases across the transition the first derivative of \( \sigma_{xy} \) is positive and if the Chern number decreases the derivative is negative. The change is small and the features in the first derivative are also small (we have multiplied \( \sigma_{xy} \) and \( \sigma_{xy}' \) by a factor of 10).

A much stronger signal is provided by the second derivative. At a transition where the Chern number changes, the second derivative exhibits two close peaks: a negative peak followed by a positive one when the Chern number increases (and vice versa if the Chern number decreases).

We note that this asymmetry of the two close peaks is a distinct feature of the topological transition. If the gap closes and \( C \) does not change, the second derivative displays a symmetric feature. Even though fig. 3 shows the particular case of \( p \)-wave pairing with strong SO coupling, we found similar behavior for weak SO coupling in the unitary and non-unitary regimes, as well as for \( s \)-wave, \( s + id \) and \( d + id \) pairings.

For this reason we believe the present behavior of \( \sigma_{xy} \) is robust and may be interpreted as follows. In the case of a topological insulator, the derivative is a Dirac delta function and the second derivative is the derivative of a Dirac delta function. In the TSC these delta functions are smeared but are still clear evidence of the location of the transition and, moreover, of the change in the topological number. The sharp features in the derivatives of \( \sigma_{xy} \) are thus reminiscent of the derivatives of the step function behavior that occurs in an insulator.

**Edge states.** — Due to the bulk-edge correspondence, complementary information on the topological phases and transitions may be obtained by analyzing the edge states. We consider a strip geometry of transversal width \( N_y \) and apply periodic boundary conditions along the longitudinal direction, \( x \). The spectrum includes states in the bulk and states along the edges.

**Strong SO coupling.** — In the case of strong SO coupling with \( M_z = 0 \) the system belongs to the symmetry class DIII [36,37]. In the \( s \)-wave case there is only the bulk gap and no gapless (edge) states. This is a topologically trivial phase. In the case of \( p \)-wave pairing, even though the Chern number vanishes there are gapless edge states [22]. The system is in a \( Z_2 \) topological phase. Because of TRS, Kramers pairs of edge states, which are counterpropagating, give opposite contributions to the total Chern number, \( C = 0 \). This is a similar situation to that in the spin Hall effect, where, even though the charge current vanishes, there is a spin current along the edges. In the case where there is a mixture of \( s \)- and \( p \)-wave components and the amplitude of the \( p \)-wave pairing is larger than the corresponding amplitude of the \( s \)-wave case, there are edge states and a topologically non-trivial phase. Because of spin-momentum locking there is no backscattering and these states are topologically protected from non-magnetic impurities.
As the magnetization is turned on, TRS is broken and the system’s symmetry class changes to D [36,37]. For small magnetization the $Z$-TSC is in a trivial phase with Chern number $C = 0$. It is interesting to note that even though the system is in a $C = 0$ phase the number of edge states is two; the same as that in the parent $\mathbb{Z}_2$ phase, when $M_z = 0$ [22]. For $M_z \neq 0$, however, TRS is broken and these edge states are not topologically protected against (any type of) disorder (except if $\alpha = 0$, when spin is conserved). In this sense, the system is in a trivial phase, in accordance with the Chern number $C = 0$. Nevertheless, in the clean limit these edge modes could be detected.

As the magnetization is increased a topological transition to a phase with non-zero Chern number happens for both the $p$-wave and the $s$-wave cases [22]. The sequence of Chern numbers is clearly correlated with the number of pairs of edge states as shown in ref. [22].

The presence of edge modes induced by bulk topology can also be shown using dimensional reduction and thereby calculating the winding number [41]. For $k_y = 0$ or $\pi$, the Hamiltonian $H(k)$ has the chiral symmetry: $\Gamma H(k) \Gamma^\dagger = -H(k)$, with $\Gamma = \tau_x \otimes \sigma_0$, where $\sigma_0$ is the identity in spin space and $\tau_x$ acts on the particle-hole space. The operator that diagonalizes $\Gamma$ is $[32,42] T = \sigma_0 \otimes e^{i\pi z y}$, and the Hamiltonian can be brought to the off-diagonal form: $T H(k) T^\dagger = q(k) \sigma^+ + q^\dagger(k) \sigma^-$, if $k_y = 0$, $\pi$ and $d_z = 0$ (see footnote $^2$). The winding number is then defined as $I(k_y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \text{Tr}[\Gamma^{-1}(k) \partial_{k_y} q(k) - (q^\dagger)^{-1}(k) \partial_{k_y} q^\dagger(k)]$. Physically, a non-zero $I(k_y)$ means that if the system is infinite along the $y$-direction and finite along $x$, there will be edge states with $k_y = 0$ or $\pi$ [43]. The calculation of the winding number gives the number of gapless edge modes both when the Chern number vanishes and when the Chern number is finite [22].

**Weak SO coupling.** If the pairing vector $d$ is not aligned with the SO vector, the connection between the Chern number and the number of gapless edge states is less transparent. Figure 4 shows the low-lying energy modes in the unitary case for different values of the SO coupling, $\alpha$. For the top panel $C = 0$ holds while the bottom panel $C = 2$. Even though changing $\alpha$ should not change the topology, various gapless states seem not to follow the bulk-edge correspondence. The winding number shows that the number of gapless edge modes is independent of $\alpha$, and for $C = 0$ we get $I(0) = 2$ and $I(\pi) = 0$, while for $C = 2$ we get $I(0) = 1$ and $I(\pi) = 1$.

The bulk-edge correspondence is further elucidated in fig. 5. Careful analysis shows that some of the gapless edge states do not originate from bulk topology and that the number of topologically induced edge states (given either by the winding number or the Chern number in the case of $C \neq 0$) is consistent. Only the bands of edge states that connect the upper and lower bulk bands can be traced back to the non-trivial bulk topology [44]. In fig. 5 these
d2

\[ q(k) = (\epsilon_0 + i d \sin k_x) \sigma_0 - M_z \sigma_y - (\alpha \sin k_x + i \Delta_0) \sigma_y. \]

\[ \begin{align*}
\alpha &= 0.1, \\
\alpha &= 0.3, \\
\alpha &= 0.5, \\
\alpha &= 0.7, \\
\alpha &= 0.9
\end{align*} \]

Fig. 4: Gapless edge modes in the unitary case for $C = 0$ (top) and $C = 2$ (bottom). Here $\epsilon_F = -1, d = 1$ and $M_z = 0.5$ (top), $M_z = 1.2$ (bottom).

\[ \begin{align*}
\alpha &= 0.1, \\
\alpha &= 0.3, \\
\alpha &= 0.5, \\
\alpha &= 0.7, \\
\alpha &= 0.9
\end{align*} \]

Fig. 5: (Color online) Gapless edge modes in the unitary case for $C = 0$ (left) and $C = 2$ (right). Here $\epsilon_F = -1, d = 1$ and $M_z = 0.5, \alpha = 2$ (left), and $M_z = 1.2, \alpha = 3$ (right).

correspond to colored lines connecting negative and positive bulk bands; clearly, the leftmost and rightmost edge state bands in the first panel do not satisfy this prescription. Denoting the two edges of the system as $R$ and $L$ in fig. 5, where $R$ is red (black) and $L$ is blue (gray), we see that for $C = 0$ the number of propagating states at each edge is always the same as the number of counter propagating ones. For $C = 2$, on the other hand, the difference between propagating and counter propagating states is always 2 at each edge.

**Non-trivial topology in normal phase.** We may as well consider a system that is non-trivial in the normal phase and add superconductivity either self-consistently or via the proximity effect [20].

Considering a Hamiltonian of the form $\hat{H}(h) = h(k) \cdot \tau + h_0(k) \gamma_0$, where $h = (h_x, h_y, h_z)$, $\tau$ are Pauli matrices and $\gamma_0$ is the identity, and selecting $h_x = \alpha \sin k_y$, $h_y = -\alpha \sin k_x$, $h_z = 2t_1 (\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y$, leads to non-trivial phases as the hoppings $t_1$ and $t_2$ are varied [45]. In the normal phase TRS is broken since $h_z$ is even in the momentum. The Chern number is $C = 2$ if $|t_1| < |t_2|$, and $C = 1$ if $|t_1| > |t_2|$. As the system becomes superconducting, the non-trivial topology remains even though the Chern number changes. The non-trivial topology of the normal state lends some robustness to the TSC phase. Indeed, the Chern number remains invariant in large portions of the parameter space. For negative
chemical potential the Chern number is \( C = -3 \) except for some narrow regions where \( C = 5 \). For zero and positive chemical potential there is a single topological transition from \( C = -3 \) to \( C = -1 \). We have checked that there is a clear correspondence between the Chern number and the number of gapless modes. We have also checked that \( \sigma_{xy} \) also signals the topological transitions.

**Conclusions.** Unlike the case of an anomalous Hall insulator, where \( \sigma_{xy} \) is quantized and its discontinuous changes clearly signal topological transitions, \( \sigma_{xy} \) in a SC is not quantized [46]. We have, nevertheless, shown that \( \sigma_{xy} \) and its derivatives may be used to detect the topological transitions that occur in Z-TSCs. This provides a bulk detection method of these transitions that is complementary to the detection of the gapless edge states associated with these non-trivial topological phases.

In the case of strong SO coupling there is a simple correspondence between the number of gapless edge states and the Chern number, both for trivial and non-trivial normal state bands. However, in the case of weak SO coupling where the pairing vector, \( d \), is not parallel to the SO vector, \( s \), extra unprotected gapless modes appear. The bulk-edge correspondence is preserved as evidenced by the calculation of the winding number.

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