Helical edge states induced by lateral spin-orbit coupling

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I. INTRODUCTION

In contrast to quantum Hall systems, dissipationless edge states can be realized in 2D topological insulators (TIs) without the need of an external magnetic field. In 2D TIs, such as inverted HgTe/CdTe and inverted InAs/GaSb quantum wells, the TI phase (also known as a quantum spin Hall insulator) is characterized by the existence of gapless, topologically protected helical edge states whose energies cross the bulk energy gap. The edge channels consist of counterpropagating states with opposite spins. Since one of the edge states is the time-reversal reversal of the other, backscattering due to time-reversal symmetric perturbations emerge, and the system behaves as a 2D topological insulator (TI). However, unlike in previous works on TIs, the mechanism proposed here for the creation of protected helical edge states relies on the strong edge SOC rather than on band inversion.

II. THEORETICAL MODEL

We consider a heterostructure in which a two-dimensional electron gas (2DEG) is confined inside a symmetric quantum well (QW) of width \( d \) grown along the \( \hat{z} \parallel [001] \). The quantum well is assumed to support a single bound state with energy \( \epsilon_z \). In addition, the step-like potential \( V_{\text{edge}}(x) \) defines the edges (located at \( x = 0 \) and \( x = L \)) of the 2DEG along the \( \hat{x} \parallel [100] \) direction (see Fig. 1). When the distance, \( L \), is large enough, the overlap between the wave functions localized at different edges can be neglected and each edge can be treated independently from the other. In such a case it suffices to analyze one of the edges, say the edge at \( x = 0 \). In the vicinity of the edge at \( x = 0 \) the in-plane motion of the 2DEG is described by the effective 2D Hamiltonian

\[
H_{2D} = p_x \left[ \frac{1}{2m^*(x)} p_x \right] + \frac{p_y^2}{2m^*(x)} + V_0 \Theta(-x) + \epsilon_z + \frac{\alpha}{\hbar} \delta(x)p_y \sigma_z - \gamma \delta(x),
\]

where \( p_x \) (\( p_y \)) is the \( x \)-component (\( y \)-component) of the momentum, \( \sigma_z \) is a Pauli matrix, \( V_0 \) is the height of the potential barrier at the edge, and \( \delta(x) \) and \( \Theta(x) \) denote the Dirac delta and unit step functions, respectively. The effective mass takes the values \( m^* = m_{\text{in}} \) and \( m^* = m_{\text{out}} \) in the regions \( x > 0 \) and \( x < 0 \), respectively. The presence of the edge at \( x = 0 \) locally breaks the structure inversion symmetry in the \( x \) direction. This gives rise to the edge SOC, which is described by the fifth term on the right-hand-side of Eq. (1) and has an amplitude \( \alpha \). The last term accounts for the possible existence of localized Tamm-like edge states. The effects of the edge SOC (also referred as lateral SOC in the case of quantum wires) on the spin Hall effect and spin polarization in quantum wires and quantum point contacts have been investigated from both the theoretical and experimental points of view. Spin-dependent scattering of bulk-like states caused by the edge SOC in a 2DEG as well as the formation of interface states in 2DEGs with position-dependent Rashba and Dresselhaus SOC have also been theoretically investigated.
According to Eq. (1) both the $y$-component of the momentum and the $z$-component of the spin remain as good quantum numbers. The eigenfunctions of $H_{2D}$ can then be written as

$$\Psi_\sigma(x, y) = \frac{1}{\sqrt{I}} e^{ik_y y} \psi_\sigma(x) \chi_\sigma, \tag{2}$$

where $l$ is the length of the sample in the $y$ direction and $\chi_\sigma$ denotes the eigenspinors of $\sigma_z$ with $\sigma = 1$ and $\sigma = -1$ for up and down spins, respectively. The functions $\psi_\sigma(x)$ obey the effective Schrödinger equation,

$$\left\{ p_x \left[ \frac{1}{2m^*(x)} p_x \right] + V_\sigma(x) \right\} \psi_\sigma(x) = \epsilon_\sigma \psi_\sigma(x), \tag{3}$$

with the spin-dependent effective potential,

$$V_\sigma(x) = V_{1D} \Theta(-x) + (\sigma \alpha k_y - \gamma) \delta(x), \tag{4}$$

and $V_{1D} = V_0 - (1 - r_m) \epsilon_y$. Here we introduced the effective mass ratio $r_m = m_{in}/m_{out}$. The eigenenergies, $\epsilon_\sigma$, are measured with respect to the value $\epsilon_y + \epsilon_z$, where $\epsilon_y = \hbar^2 k_y^2 / (2m_y)$.

In samples with symmetric edges, the wave functions, $\Psi^{(L)}_\sigma(x, y)$, localized around the edge at $x = L$ can be obtained from those localized around $x = 0$ [see Eq. (2)] by using the symmetry relation, $\Psi^{(L)}_\sigma(x, y) = \Psi_{-\sigma}(L - x, y)$. We first consider the case in which the edge states are induced exclusively from the edge SOC and take $\gamma = 0$. In such a case, the origin of the SOC-induced edge states can be qualitatively understood by analyzing the effective edge potential $V_\sigma$. The first term in the right-hand-side of Eq. (4) represents an effective potential barrier at the edge while for $\gamma = 0$ the second term can be attractive or repulsive in dependence of whether the sign of the product $\sigma \alpha k_y$ is negative or positive [see Figs. 2(a) and (b)]. Therefore, assuming that the constituent materials are such that $\alpha > 0$ (the generalization to the case $\alpha < 0$ is straightforward), the spin-dependent potential $V_\sigma$ forms an asymmetric QW for both spin-up ($\sigma = 1$) carriers with $k_y < 0$ and spin-down ($\sigma = -1$) carriers with $k_y > 0$, as schematically shown in Fig. 2(a). Since the resulting edge QW is asymmetric, it does not support bound states for arbitrary values of $k_y$. However, bound states can emerge when $|k_y|$ is larger than a certain critical value. These bound states are localized in the $x$ direction around the edge but propagate freely in the $y$ direction. They represent two counterpropagating spin-polarized edge channels with opposite spin polarization, one of which is the time reversal of the other [see Fig. 2(c)]. Note that the net spin polarization vanishes, as dictated by the time-reversal invariance of the Hamiltonian in Eq. (3). In a nonequilibrium situation, however, the edge SOC can lead to spin-dependent scattering of bulk-like states at the edge and produce a finite spin polarization.

![Figure 2](image_url)

**FIG. 2.** (Color on line). Formation of edge states. In the presence of the edge SOC, the effective edge potentials become spin-dependent. Close to the edge at $x = 0$ the potential is attractive (a) or repulsive (b) in dependence of whether the product $\sigma \alpha k_y$ is negative or positive. When the potential is strong enough, localized edge states can emerge. For $\alpha > 0$, $V_\sigma$ is attractive for spin-up ($\sigma = 1$) carriers with $k_y < 0$ and spin-down ($\sigma = -1$) carriers with $k_y > 0$. This leads to the formation of two counterpropagating edge states with opposite spins. The effective edge potential at $x = L$, $V^{(L)}_\sigma(x) = V_{-\sigma}(L - x)$. Therefore, edge states similar to those at $x = 0$ also appear at $x = L$ but with inverted spins. (c) Schematic of the spin-polarized, counterpropagating edge states. At equilibrium, the finite spin currents flowing along different edges compensate each other and the total spin current vanishes.

The eigenenergies and eigenfunctions of Eq. (3) corresponding to bound states are given, respectively, by

$$\epsilon_\sigma = -\frac{\hbar^2 k_y^2}{2m_{in}}, \tag{5}$$

and

$$\psi_\sigma(x) = \sqrt{\frac{2\kappa_\sigma k_y}{\kappa_\sigma + k_y}} \times \left\{ e^{\kappa_\sigma x}, \quad x < 0 \right\} e^{-k_y x}, \quad x \geq 0, \tag{6}$$

where $\kappa_\sigma = \sqrt{(k_y^2 + q_0^2)/r_m}$ and $q_0 = \sqrt{2m_{in} V_{1D}/\hbar^2}$. The wavevector $k_y$ obeys the dispersion relation

$$k_y = \sqrt{r_m(k_y^2 + q_0^2) + \sigma \lambda \alpha k_y}, \tag{7}$$

where $\lambda = 2m_{in} \alpha / \hbar^2$ is a dimensionless parameter characterizing the strength of the edge SOC. In what follows we shall focus in the case $m_{out} > m_{in} > 0$ and
assume that \( q_0 \) is real. The other cases can be treated in a similar way.

For Eq. (7) to represent bound states, \( k_\sigma \) must be a positive real number and therefore the appropriate solutions of Eq. (7) reduce to the form

\[
    k_\sigma = \frac{-\sigma \lambda_{SO} b}{\lambda_{SO}^2 k_y^2 + m(1-r_m)q_0^2} + \frac{1}{1-r_m},
\]

where \( 0 < r_m < 1 \). The requirement that \( k_\sigma \) must be a positive real number imposes constraints to the existence of the solutions in Eq. (7). For example, if \( \lambda_{SO} > 0 \) \((\lambda_{SO} < 0)\) a necessary, although not sufficient, condition for the existence of bound states is \( \sigma k_y < 0 \) \((\sigma k_y > 0)\), as inferred from Eq. (8). This confirms our early argument that the SOC-induced edge states represent two spin-polarized counterpropagating channels with opposite spins.

On the other hand, positive real values of \( k_\sigma \), and therefore edge states, do not exist for arbitrary values of \( k_y \) but only for those values for which the first term in the numerator in Eq. (8) becomes larger than the second one. A more general analysis of Eq. (8) reveals that if the SOC strength is such that \( \lambda_{SO}^2 < (1-r_m) \), the domain of \( k_y \) values for which edge states exist is given by

\[
    \frac{r_m b}{r_m(1-r_m) + \lambda_{SO}^2} < (k_y d)^2 < \frac{b}{(1-r_m) - \lambda_{SO}^2}. \tag{9}
\]

On the other hand, if \( \lambda_{SO}^2 > (1-r_m) \) the \( k_y \)-domain for edge states is

\[
    (k_y d)^2 > \frac{r_m b}{r_m(1-r_m) + \lambda_{SO}^2}. \tag{10}
\]

In the equations above the dimensionless parameter \( b = V_0/\epsilon_0 \) characterizes the height of the edge potential in units of the energy \( \epsilon_0 = \hbar^2/(2m_\sigma d^2) \).

In contrast to the edge states of the integer quantum Hall phase and/or in inverted band 2D topological insulators the edge states induced by the edge SOC are, in general, not protected against disorder. This is so because although scattering from one edge state to the other is forbidden by time reversal symmetry, backscattering can occur through the bulk-like states which, in general, coexist with the edge states in the same energy range. However, protected edge states may appear in gapped materials with strong enough edge SOC. In such a case edge states can exist inside the band-gap and be energetically isolated from the bulk-like states, as will be shown below.

The band gap of the material forming the 2DEG is located below the ground state energy of the QW, \( \epsilon_z \). In order to induce bound states inside the gap, the SOC strength must be such that the total energy of the edge states, \( E_\sigma = \epsilon_\sigma + \epsilon_y + \epsilon_z \), becomes smaller than \( \epsilon_z \), i.e., the condition

\[
    \epsilon_\sigma + \epsilon_y = \frac{\hbar^2}{2m_\sigma} (k_y^2 - k_\sigma^2) < 0 \tag{11}
\]

must be satisfied. This condition imposes an additional constraint for the edge states to be protected against time-reversal invariant perturbations. Using Eqs. (8) and (11) one finds that a necessary condition for the emergence of protected edge states is,

\[
    |\lambda_{SO}| > 1 + r_m. \tag{12}
\]

When the edge SOC is weak, Eq. (12) is not fulfilled and only unprotected edge states exist. However, when the edge SOC is strong enough and Eq. (12) is satisfied, the dissipationless edge states emerge in the \( k_y \)-domain specified by

\[
    |k_y d| > \sqrt{\frac{r_m b}{\lambda_{SO}^2 - r_m^2}}. \tag{13}
\]

### III. RESULTS

The emergence of the helical edge states computed for \( r_m = 0.2 \) and \( V_0/\epsilon_0 = 100 \) is displayed in Fig. 3(a), as a function of the spin-orbit parameter \( \lambda_{SO} \) and the momentum. The white zones correspond to the absence of edge states, while the red and sparse blue regions correspond, respectively, to unprotected and protected helical edge states. The uparrows (downarrows) indicate that the spin orientation of the states in the corresponding quadrants is parallel (antiparallel) to the \( \mathbf{z} \) direction. As discussed above, at \( \lambda_{SO} = 0 \) there are no edge states. However, when \( |\lambda_{SO}| \) starts to deviate from zero, unprotected helical edge states emerge in a reduced region of the \( k_y \)-space. As \( |\lambda_{SO}| \) increases, the domain of the \( k_y \)-space corresponding to unprotected edge states become wider and when the condition in Eq. (12) is fulfilled, the protected edge states start to appear. The energy dispersions of the edge states corresponding to lines (1) and (2) in Fig. 3(a) (i.e., for \( \lambda_{SO} = -1, -2 \)) are shown in Fig. 3(b), where the energy of the spin-degenerate bulk-like states (dash-dotted line) has also been included for comparison. The spin orientation of the different energy branches is indicated by the arrows. The pair of helical edge states labeled by (1) coexists with the bulk-like states and is therefore not protected against disorder (backscattering can occur through transitions from the edge states to the bulk-like states). On the other hand, the helical edge states labeled by (2) enter into the gap region \((E-\epsilon_z < 0)\). Being isolated from the bulk-like states these two counterpropagating spin polarized states, one of which is the time reversal of the other, become protected against time-reversal perturbations.

The penetration of the protected edge states into the gap region can be easily understood in the extreme case \( r_m \ll 1 \) (i.e., \( m_{out} \gg m_{in} \)). In such a case Eq. (8) can be approximated by \( k_\sigma \approx -\sigma \lambda_{SO} k_y \) and yields,

\[
    E_\sigma - \epsilon_z \approx \frac{\hbar^2 k_y^2}{2\mu}, \tag{14}
\]
Thus, if \(|\lambda_\omega| > 1|\) [note that for \(r_m \to 0\), this is consistent with Eq. (12)], the mass \(\mu\) changes sign and the subbands start to penetrate into the gap region.

In the 2D TIs relying on band inversion the protected edge states form a Dirac point inside the energy gap and the corresponding energy spectrum is almost linear. In contrast, as shown in Fig. 3 (b), the protected edge states induced purely by the edge interface SOC do not form a Dirac point and exhibit a strongly non-linear spectrum. A similar behavior of the energy dispersion has also been found for the edge states in Bi(111) ultrathin films.21-22

We now consider the case \(\gamma \neq 0\) and conveniently introduce the dimensionless parameter \(q = 2m_in_Gd/\hbar^2\). As long as the inequality \(0 < q < \sqrt{\gamma m_G}(k_y = 0)\) holds, there are no qualitative differences to the case \(q = 0\). The only effect is the reduction of the \(k_y\)-domain in which edge states do not exist [i.e., the white zones in Fig. 3 (a)] are reduced when increasing \(q\). This is because as \(q\) increases, the energy branches corresponding to the counterpropagating edge states tend to match each other at the zone center. If the value of \(q\) is such that \(q > \sqrt{\gamma m_G}(k_y = 0)\), a Dirac point at \(k_y = 0\) emerges inside the energy gap and helical Tamm-like edge states appear. The energy dispersion of these states is shown in Fig. 4 for \(q = 6\) [for \(r_m = 0.2\) and \(V_0/\epsilon_0 = 100\) one finds \(\sqrt{\gamma m_G}(k_y = 0) = 4.47\)]. Unprotected and protected helical Tamm-like edge states are represented, respectively, by solid lines in Figs. 4 (a) and (b). The dash-dotted lines describe the bulk-like states and the arrows indicate the spin orientation of the corresponding energy branch. The unprotected edge states exhibit a typical Rashba-type spectrum [see Fig. 4 (a)]23 while the energy spectrum of the protected edge states [see Fig. 4 (b)] resembles that of an inverted band TI.

**IV. CONCLUSIONS**

Protected edge and surface states are known to appear in systems with strong atomic SOC in which a band inversion drives the system into a topological insulator phase.11-12 The mechanism proposed in this work does not rely on band inversion but rather on the use of the edge SOC. It represents a new alternative for the creation of protected helical edge states that could be relevant for engineering new types of topological insulators. Unfortunately, although the model presented here provides a qualitative description of the formation of such states, it is difficult at the present stage to predict which materials should be combined for the condition in Eq. (12) to be fulfilled and the protected helical states to appear. This is so because the parameter characterizing the strength of the edge SOC (\(\alpha\) or its dimensionless version, \(\lambda_\omega\)) is not precisely known for much systems. In general, the value of \(\alpha\) must be extracted from first-principles calculations or deduced from experiments. Nevertheless, rough estimations of \(\alpha\) have been reported for some interfaces between III-V semiconductors.24 We have performed similar estimations for other kind of experimentally relevant interfaces between III-V semiconductors and found that for these interfaces the condition in Eq. (12) is, in general, not fulfilled. However for InSb/In_{0.65}Al_{0.35}Sb and Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As interfaces we found \(|\lambda_\omega| \sim 0.3\), a value that is only about 4 to 5 times smaller than the value required for the emergence of the protected helical edge states. This suggests that the proposed mechanism may indeed exist in other kind of edges (e.g., with
vacuum or between materials with non-common atoms) where the interface SOC can, in principle, be enhanced even by orders of magnitude.

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