Valley selecting current partition at zero-line mode of quantum anomalous Hall topologies

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Abstract

Topologically protected zero-line modes appear at the interface between two regions of the monolayer graphene in quantum anomalous Hall phase with different Chern number. In the presence of staggered sublattice potential, the band gaps of the two valleys become different, and the phase diagram defined by the Chern number has an additional regime of topologically trivial phase. The interface between the topologically trivial and non-trivial regions hosts zero-line mode in only one valley. By tuning the exchange field, three types of interface that host zero-line modes in selected valley(s) are formed. The nano-devices consisted of Y-shape junctions of the three types of interface exhibit the functions of valley splitting, merging or filtering for the incident currents.

Keywords: graphene, zero-line mode, valleytronic, valley selecting current partition, quantum anomalous Hall topologies

(Some figures may appear in colour only in the online journal)
The article is organized as following: in section 2, the tight binding model for the graphene with Rashba SOC, exchange field and staggered sublattice potential is given. The phase diagram and band structure of the bulk graphene is discussed in this section. The band structure of the ZLMs in the middle of the zigzag nano-ribbon is calculated. In section 3, the Y-shape junctions are proposed. The two devices with valley splitting (merging) and filtering effects are simulated by applying the non-equilibrium Green’s function method. In section 4, the conclusion is given.

2. Quantum anomalous Hall topologies with staggered sublattice potential

The tight binding Hamiltonian of the graphene with exchange field, staggered sublattice potential and Rashba spin-orbital coupling (SOC) is given as

\[ H = -t \sum_{\langle ij \rangle, \alpha} c_{i\alpha}^+ c_{j\alpha} + ig_\lambda \sum_{\langle ij \rangle, \alpha, \beta} c_{i\alpha}^+ (S \times d_{ij}) \cdot \hat{\pi}_{\alpha \beta} c_{j\beta} + \lambda \sum_{i, \alpha} c_{i\alpha}^+ \sigma_z c_{i\alpha} + \Delta \sum_{i, \alpha} \delta_{\alpha} c_{i\alpha}^+ c_{i\alpha} \]

(1)

where \( i \) and \( j \) label the lattice sites, \( \alpha = \pm 1 \) and \( \beta = \pm 1 \) label the spin, the summations with index \( \langle ij \rangle \) run through the nearest neighboring sites, \( t = 2.8 \text{eV} \) is the nearest neighbor hopping energy, \( g_\lambda \) is the Rashba SOC strength, \( \lambda \) is the exchange field strength, \( \Delta \) is the staggered sublattice potential, \( \delta_{\alpha} = +1(-1) \) for \( \alpha = 1(2) \), \( S = \{\sigma_x, \sigma_y, \sigma_z\} \) is vector of Pauli matrixes, \( d_{ij} \) is the unit vector from lattice \( i \) to \( j \).

Applying the Bloch periodic boundary condition, the bulk band structure is obtained. The topological phase is determined by the Chern number (denoted as \( \hat{C} \)), which is the integral of the Berry curvature through the whole Brillouin zone. The phase diagram is plotted in figure 1(a). The phase transition boundaries are featured by gap closing, which occur at K or K’ point. In the simultaneous presence of the staggered sublattice potential and exchange field, the band structures in K and K’ valley are different. Specifically, the eigenvalues at K(K’) point are \( \pm(\Delta - (+)\lambda) \) and \( \pm(\Delta + (+)\lambda)^2 \). In the regime with \( \lambda > (\Delta - 2g_\lambda^2/(4\Delta)) \) (to the left of the dash line in figure 1(a)), the band gap at K(K’) point is \( 2\sqrt{g_\lambda^2 + (\Delta - (+)\lambda)^2} \); in the other regime, the band gap at K(K’) point is \( 2\Delta - (+)\lambda \). Thus, the band gap at K(K’) point is closed when \( \lambda = -2\Delta \) or \( g_\lambda = 0 \) and \( \lambda = +2\Delta \). The global band gap is close at two solid lines in figure 1(a), which separate the topological trivial and non-trivial phases.

The band structures of three typical systems with parameter being labeled in figure 1(a) are plotted in figures 1(b)-(d), respectively. In the trivial phase with \( \lambda = 0 \), the band structures of K and K’ valleys are the same, as shown in figure 1(b).

The band gap is 2\( \Delta \). Increasing \( \lambda \) drives the band gap in K(K’) point smaller (larger). The Berry curvature of a system in this phase regime is plotted in figure 2(a). The Berry curvature in K and K’ valley have opposite sign. The integral of the Berry curvature through the whole Brillouin zone gives \( \hat{C} = 0 \). With \( \lambda = \Delta \), the gap at K point is closed, as shown in figure 1(c). By contrast, with \( \lambda = -\Delta \), the gap at K’ point is closed. This critical phase is valley-polarized semi-metal. Further increasing \( \lambda \) reopen the gap at K point. The Berry curvature of a system in this phase regime is plotted in figure 2(b). In this case, the Berry curvature in K and K’ valley have the same sign. The integral of the Berry curvature through half of the Brillouin zone that cover one valley gives fractional number. The integral of the Berry curvature through the whole Brillouin zone gives \( \hat{C} = \pm 4 \). With \( \lambda = 2\Delta \), the band gap at K point reaches 2\( \Delta \) again, as shown in figure 1(d). Note that the global band gap is slightly smaller than 2\( \Delta \), because the band minimal locates beyond the K point. Flipping the sign of the exchange field exchange the band structures at K and K’ points. As a result, the electron transportation and optical excitation in these graphenes exhibit valley selecting property that is controlled by the exchange field.

The ZLMs are formed at the interface between two regions with different Chern numbers. In order to exhibit the ZLMs numerically, we calculate the band structures of zigzag nanoribbons. The lattice structure of the nano-ribbon is plotted in figure 3. The domain wall is located in the middle of the nano-ribbon along the longitudinal direction (x axis). When the exchange fields to the left and right of the domain wall are \( \lambda = +2\Delta \) and \( \lambda = -2\Delta \), respectively, the band structure is shown in figure 4(a). The ZLMs at the two valleys have the same dispersion, so that the localized conductivity of the ZLMs is finite (zero) under forward (backward) bias, assuming that the Fermi level is in the bulk gap and crosses the dispersion of the ZLMs. In addition to the ZLMs, the
chiral edge states localized at the left and right open edges are also gapless. The dispersion of the chiral edge state is opposite to the dispersion of the ZLMs. If the $y$ coordinate of the domain wall is changed by $\frac{N}{a}$, with $a$ being the bond length of graphene and $N \in \{\pm 1, \pm 2, \pm 3\}$, the domain wall cuts through different types of bond. The dispersions of the ZLMs would be slightly changed, but the topological features remain the same. If the domain to the right of the domain wall has zero exchange field, the ZLMs in the $K$ valley disappear, as shown in figure 4(b). Meanwhile the edge states localized at the right open edges become two-fold degenerated flat band. The energy of the flat band is equal to the local potential of the edge atoms. By contrast, if the domain to the left of the domain wall have zero exchange field, the ZLMs in the $K'$ valley disappear, as shown in figure 4(c). Thus, the numerical results of the band structures confirm that the number of gapless edge states at the interface between two regions is determined by the difference between the Chern numbers of the two adjacent regions.

In the presence of electron–electron interaction, the band gap would be modified, but the topological number remains the same in this case. The interaction is described by the additional term of Hubbard model, $U \sum_i \hat{n}_{i,\alpha} \hat{n}_{i,\alpha}$, in the Hamiltonian of the tight binding model. In our calculation, the realistic parameter with $U = 1.6t$ is used. The model can be solved by the cluster perturbation theory (CPT) method [38–42], which gives the spectral function. The spectral function is the LDOS at each lattice site versus the energy and wavenumber. Summation of the spectral function at the lattice sites around the domain wall or the open edges shows the quasi-particle dispersion of the corresponding edge states. For the nano-ribbons with parameter in figure 4(a), the summations of the spectral function around the left open edge, the domain wall and the right open edge are plotted in figures 4(d)–(f), respectively. The band structures of the chiral edge states and ZLMs without interaction is plotted in the corresponding figures for comparison. In figures 4(d) and (f), within the energy range of the bulk gap, one can find that the dispersions of the chiral edge states are not significantly modified by the interaction. In figure 4(e), one can find that the momentum difference between the two ZLMs in the same valley is enlarged due to the interaction. For the nano-ribbon with parameter in figure 4(c), the summations of the spectral function around the left open edge, the domain wall and the right open edge are plotted in figures 4(g)–(i), respectively. In figure 4(i), one can find that the flat bands at the open edge of the region with $C = 0$ is moved toward $\varepsilon = 0$ due to the interaction. The flat band become slightly dispersive with finite conductivity under forward and backward bias. Because the Hubbard interaction does not qualitatively change the conductive properties around $\varepsilon = 0$, the non-interacting model is used in the following sections.

3. Valley splitting current partition

Because changing the exchange field drives the graphene into three topological phase with different Chern number, the interfaces between any two phases support three types of ZLM. The Y-shape junction of three ZLMs has the function of current partition. We denote the three type of ZLMs in figures 4(a)–(c) as ZLM-a, ZLM-b and ZLM-c.

The nano-structure with valley splitting effect is presented in figure 5(a). Because the ZLM-b and ZLM-c only support current in $K$ and $K'$ valley, respectively, under forward bias, the incident charge current from the ZLM-a are split into two currents. Because all ZLMs have positive dispersion, the backward bias does not excite current in the ZLMs, but excite currents along the open edges. Flipping the sign of the exchange field at all regions gives the nano-structure with valley merging effect, as shown in figure 5(b). In this case, the forward bias excite currents along the open edges;
The backward bias excite valley polarized current at ZLM-b and ZLM-c, which merge at the Y-shape junction. The proposal are confirmed by numerical calculation of quantum transportation based on the non-equilibrium Green’s function (NEGF) theory [43–47]. The recursive algorithm is applied to construct the Green’s function. The local density of state (LDOS) is given by the imaginary part of the retarded Green’s function as $-\frac{1}{\pi} \text{Im}[G^r(r)]$. The local current is given as

$$j(r_i \rightarrow r_j) = \frac{2e}{\hbar} \int dE \left[ t_{ij} G^< (r_i, r_j) - t_{ji} G^< (r_j, r_i) \right]$$  \hspace{1cm} (2)$$

where $r_i$ is the position of the $i$th lattice site, $\hat{d}_{ij}$ is the unit vector from the $i$th to $j$th lattice site, $e$ is the electron charge, $\hbar$ is the Planck constant, $t_{ij}$ is the hopping parameter between the $i$th and $j$th lattice site, and $G^<(r_i, r_j)$ is the lesser Green’s function. For the system in figure 5, the front and back leads are the nano-ribbons with one and two domain walls, respectively; the Y-shape junction is the scattering region. The numerical results are plotted in figures 5(c) and (d) for the Y-shape junction in figures 5(a) and (b), respectively. Both figures present the results with forward bias. Under backward bias, the current distributions of the system in figures 5(a) and (b) are given by the result in figures 5(d) and (c) with reversing current direction, respectively. The results show that the system in figure 5(a) has valley splitting effect under forward bias. In contrary, the system in figure 5(b) has valley merging effect under backward bias.

Although the ZLM-a support current in both valley, excitation of valley polarized current in ZLM-a could be useful for valleytronic devices. The valley filtering devices consisting of two Y-shape junction is presented in figures 6(a) and (b). The background of the nano-structure is the nano-ribbon with ZLM-a. In the scattering region, the exchange field in a square panel is switched to $\lambda = \pm 2\Delta$. The total width of the nano-ribbon is 51.12 nm. The bands of the ZLMs are plotted as black (solid) lines, the bands of the chiral edge states at the left open edge are plotted as red (dotted) lines and the bands of the chiral edge states at the right open edge are plotted as blue (dashed) lines. The thick red (solid) and blue (dashed) lines are the bulk band edge of the left and right regions, respectively. The thin black (solid) lines are bulk states. In the presence of the Hubbard interaction, the spectral function of the system with parameters in (a) are plotted in ((d)–(f)). Specifically, the summations of the spectral function around the left open edge, the domain wall and the right open edge are plotted in (d)–(f), respectively. The non-interacting band structures of the corresponding chiral edge states or ZLMs are plotted as thin lines for comparison. Spectral functions of the same scheme are plotted in ((g)–(i)) for the system with parameters in (c).
Figure 5. (a) and (b) are spatial blueprint of the Y-shape junction in a nano-ribbon. The exchange fields of each region in (a) and (b) are labeled in the figures. The black arrow indicate the localized edge states (ZLMs or chiral edge states) that support current in both valley, the white (grey) arrow indicate the localized edge states that support valley polarized current in K(K’) valley. (c) and (d) are the numerical result of the transportation calculation of the systems in (a) and (b) under forward bias, respectively. The color scale indicates the LDOS, and the vector fields indicates the local current distribution.

Figure 6. The same type of plotting as in figure 5 for the valley filtering devices. In (a) and (b), the wider black arrow indicate the incident charge current; the wider white (grey) arrow indicate the exiting valley polarized current at K(K’) valley at the ZLMs that support current in both valley.
4. Conclusion

In summary, the ZLMs at the domain walls of monolayer graphene are studied. If the domain wall separates two regions in QAH phase with opposite Chern number, the ZLMs support one-way current in both K and K′ valleys; if the domain wall separates the region in QAH phase from the region in topologically trivial phase, the ZLMs support one-way current in either K or K′ valley. The Y-shape current partition at the junction of three different type of ZLMs are proposed. The devices with valley splitting, merging and filtering effects are designed. The valley filtering device makes integrated valley-tronic feasible.

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around \( \varepsilon = 0 \) at the open edge of the square panel is near to zero, this section of the open edge does not support current. For the system in figure 6(a), under forward bias, the incident port excite current along the ZLM-a in both of the K and K′ valleys. At the first Y-shape junction, the K valley current is partitioned into the ZLM-c (parallel to the nano-ribbon) in the scattering region, while the K′ valley current is partitioned into the ZLM-b (perpendicular to the nano-ribbon). At the second Y-shape junction, the K valley current transmits into the ZLM-a of the exiting port. The K′ valley current is redirected into the open edge and flow back to the incident port. The devices effectively transmit the K valley current and reflect the K′ valley current, which form the K valley filter. Similarly, the system in figure 6(b) form the K′ valley filter. The proposal is confirmed by the quantum transportation calculation as well, which is plotted in figures 6(c) and (d).
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