Current propagation behaviors and spin filtering effects in three-terminal topological-insulator junctions

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Abstract

Understand the spin and current behavior in the topological-insulator (TI) system is crucial for the design of electronic and spintronic devices. To study these behaviors, some three-terminal hetero-junction TI systems made from the zigzag silicene-like nanoribbons (ZSiNRs) are investigated. Different external fields are applied in the leads and conductor regions, which result in the expected topological edge states. By calculating the local current distribution, we find two important characteristics of topological edge current propagating in these systems. Firstly, the topological edge current prefers to flow into the nearest channel, rather than the other faraway channels. Secondly, the group-velocity mismatch as a scattering engineering has a significant effect on current propagation behavior. In other words, one can manipulate the topological edge current by velocity mismatch. Based on these characteristics, a type of three-terminal spin filter is proposed in this paper. Moreover, some interesting transport phenomena such as space-separated Fano-resonance are also discovered in the TI-junction systems.

1. Introduction

In recent years, the two-dimensional (2D) silicene-like materials, such as silicene, germanene, stanene, and some other silicene-derived materials [1–4], have attracted considerable interest due to its interesting properties and the compatibility with the existing semiconductor industry. Different from the weak spin–orbit coupling (SOC) and planar structure of graphene, the silicene-like materials have a strong intrinsic SOC and a low-buckled honeycomb structure [2, 5–7]. The stronger SOC makes the silicene-like materials good candidates for the topological insulator (TI) [8, 9]. And the TIs have been intensively studied due to the topologically nontrivial edge states in the absence of an external magnetic field, which is important for the development of next-generation electronic devices such as the topological transistor, spin filter, valley filter, and spin–valley filter [9–12]. For example, Zheng et al [12] proposed a topological transistor based on Xenes (X = Si, Ge, or Sn) which show features of a topological insulator. The topological transistor can be switched between on state or off state by adjusting the off-resonant circularly polarized light (induced topological phase transition).

The main property of TI is insulating in bulk states and conducting in edge states on the surface. Different TIs correspond to different topological phases, which include the quantum spin Hall effect (QSH) [1], quantum anomalous Hall effect (QAH) [13, 14], and spin-polarized quantum anomalous Hall effect (SQAH) [15]. The QSH effect has the helical edge states, where the spin-up and spin-down modes flow in the opposite directions on the upper and lower nanoribbon edges. Whereas, the QAH effect corresponds to the chiral edge state, where the spin-up and spin-down modes flow in the same upper or lower edges along the same direction. And the SQAH effect is characterized by a perfect spin-polarized state in which only a spin-up or spin-down mode flows in the opposite direction between the two edges [10, 16]. The peculiar properties of topological edge states stimulate the study of its transport property, which is a platform for designing spintronic for information processing utilizing a spin degree of freedom [10, 11, 17].
Undoubtedly, we can give better designs for spintronic devices when we understand the behavior of topological edge current in the TI system.

In this work, we design some three-terminal hetero-junction systems with the TI made from the zigzag silicene-like nanoribbons (ZSiNRs) to study the topological edge current behavior. To obtain the expected TI edge state in the leads and conductor region, three types of external fields are considered. The local current distribution is calculated to visualize the detailed transport process. We find some important features of topological edge current in these systems. First, if there are two available channels, the topological edge current has a much greater probability flow into the nearest channel than the other channel. Second, the group-velocity mismatch has a significant effect on current behavior. Based on these characteristics, a kind of three-terminal spin filter is proposed in this work. Furthermore, interesting transport phenomena such as Fano resonances are also discovered.

2. Model and methods

In this work, the three-terminal system made from the ZSiNRs consists of four parts: lead 1, lead 2, lead 3, and conductor (figure 1). The currents are incident from lead 1 and finally are transmitted into the output leads (lead 2 and lead 3). It is noted that in most of our studies the conductor is the same as lead 1 (expect contents in figure 6). They thus have the same energy band and transport properties. We use the tight-binding model for the system as below [10, 15]

\[
H = -i \sum_{\langle ij \rangle} c_{i\alpha}^\dagger c_{j\alpha} + i \frac{\lambda_{\sigma}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle} \nu_{ij} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^{\sigma} c_{j\beta} + \sum_{\alpha} E_{\alpha} c_{i\alpha}^\dagger c_{i\alpha} + \sum_{\alpha\beta} M_{\alpha\beta} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^{\sigma} c_{i\beta} + i \frac{\lambda_{\Omega}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle} \nu_{ij} c_{i\alpha}^\dagger c_{j\alpha},
\]

where \(c_{i\alpha}^\dagger\) and \(c_{i\alpha}\) are the creation (annihilation) operator of the electron with the spin \(\alpha (\alpha = \uparrow, \downarrow)\) at site \(i\) and \(i, j\) and \(i, j\) run over all the nearest and next-nearest-neighbor hopping sites. The first term denotes the nearest coupling. The second term denotes the intrinsic spin–orbit interaction. In this paper, we use some silicene-like material with \(t = 1.6\) eV and \(\lambda_{\sigma} = 0.03t\) [10]. The \(\lambda_{\sigma}\) value is close to that of germanene [15, 18]. The \(\sigma_{\alpha\beta}^{\sigma}\) is the \(z\) component of \(2 \times 2\) Pauli matrix with spin indices \(\alpha\) and \(\beta\). We set \(\nu_{ij} = -1\), when the hopping is clockwise to the positive \(z\)-axis; otherwise, \(\nu_{ij} = +1\). The third term is for the staggered electric potential with \(\mu_{ij} = \pm 1\) denoting A or B sublattice. The fourth term is the staggered exchange field which can be induced by depositing the magnetic insulators on the top and bottom of the ZSiNRs sheet with different directions [19]. The last term is the off-resonant circularly polarized light where the sign of \(\lambda_{\Omega}\) depending on the left or right circulation [10, 20]. Here we note that all these external fields are not the same in the whole parts of the TI system. In each parts of the system there may exist different external fields, which will be detailed later.
As we know, different topological phases correspond to different edge states. To explore the topological phase of these ZSiNRs, the Hamiltonian (1) is rewritten in the k-space as the function of the Bloch wave vector. Then, near the K and K′ point, we approximate the Hamiltonian in the low energy range as

\[ H'_\eta = \hbar v_F \left( \eta \tau_x k_x + \tau_y k_y \right) + (\eta s \lambda_{so} + \eta \lambda_{\Omega} + s M_{AF} + E_z) \tau_z, \] (2)

where \( v_F = \frac{\sqrt{2} \hbar \nu_F}{m} \) is the Fermi velocity with a lattice constant \( a, \eta = \pm 1 \) for K or K′ point and \( s = \pm 1 \) for spin-up or spin-down cases. \( \tau = (\tau_x, \tau_y, \tau_z) \) is the Pauli matrix of the sublattice pseudospin for the A and B sites. According to the equation (2), the spin–valley energy spectrum reads

\[ E_{\eta s} = \sqrt{(\hbar v_F k)^2 + (\Delta_\eta s)^2}. \] (3)

The gap is given by \( 2 |\Delta_\eta| \) where \( \Delta_\eta = \eta s \lambda_{so} + \eta \lambda_{\Omega} + s M_{AF} + E_z. \) The Chern number is determined by the signs of valleys and the Dirac mass: \( C_{\text{CH}} = \frac{2}{\nu_F} \text{sgn} (\Delta_\eta) \) [15]. The total Chern number \( C \) and the spin Chern number \( C_s \) are defined as \( C = C^+ + C'^+ + C^- + C'^- \) and \( C_s = C^\uparrow + C'^\uparrow - C^\downarrow - C'^\downarrow \). By calculating \( (C, C_s) \), we can obtain the topological phases of the corresponding edge states.

In the non-equilibrium Green’s function (NEG) theory, the spin-resolved transmission from lead \( i \) to lead \( j \) can be expressed as:

\[ T_{ij}^\eta(E) = \text{Tr} \left[ \Gamma_i^\eta(E) G^{\text{R},\eta}(E) \Gamma_j^\eta(E) G^{\text{A},\eta}(E) \right], \] (4)

where \( G^{\text{R},\eta}(E) \) and \( G^{\text{A},\eta}(E) \) are the retarded and advanced Green’s function with spin \( \eta \); \( \Gamma_i^\eta(E) (i = 1, 2, 3) \) is the spin-resolved linewidth function of the lead \( i \), which is defined as \( \Gamma_i^\eta(E) = i \left( \Sigma_i^{\text{R},\eta}(E) - \Sigma_i^{\text{A},\eta}(E) \right) \), where \( \Sigma_i^{\text{R},\eta}(E) \) and \( \Sigma_i^{\text{A},\eta}(E) \) are the retarded and advanced self-energy function of the lead \( i \), respectively. The retarded (advanced) Green’s function in the equation (4) is calculated as

\[ G^{\text{R(A)},\eta}(E) = \left[ (E \pm i\delta) I - H_C - \sum_i \Sigma_i^{\text{R(A)},\eta}(E) \right]^{-1}, \] (5)

where \( \delta \) is a very small positive number; \( H_C \) is the Hamiltonian of the device and \( I \) is the identity matrix with the device dimension. To study the detailed transport property of these three-terminal systems, we plot the local current in the lead and conductor regions. The energy-resolved bond current between site \( i \) and \( j \) is given below [17, 21, 22]

\[ J_{ij}^\eta(E) = H_C^j G_{ij}^\eta(E) - G_{ji}^\eta(E) H_C^i, \] (6)

where \( G^{\text{A},\eta}(E) \) is the lesser Green’s function in the energy domain expressed as

\[ G^{\text{A},\eta}(E) = -iG^{\text{R},\eta}(E)\Gamma_i^\eta(E)G^{\text{A},\eta}(E); \] (7)

and \( H_C^i \) is the relevant matrix element of the conductor’s Hamiltonian.

3. Results and analysis

3.1. Topological phase and corresponding edge state

From the Chern number formula above, we obtain the relation of the topological phase and external fields. We firstly consider only the light field term in the ZSiNRs system (width = 16). We find that if \( -\lambda_{so} < \lambda_{\Omega} < \lambda_{so} \), the topological numbers are \( (C, C_s) = (0, 1) \) or \( (0, -1) \). This is the QSH state, corresponding to the helical edge state (figure 2(a1) for the cartoon picture of edge state and figure 2(a2) for the band structure). In this work, we obtain the QSH state with the \( \lambda_{\Omega} = 0 \). Because the pristine silicene is a TI with the QSH state (helical edge state) due to the SOC effect. When \( \lambda_{\Omega} > -\lambda_{so} \), the topological numbers are \( (C, C_s) = (2, 0) \), which is a QAHE state corresponding to the chiral edge states (see figure 2(b1) for edge states and figure 2(b2) for the energy band). If \( \lambda_{\Omega} > \lambda_{so} \), we find the topological number \( (C, C_s) = (-2, 0) \) and directions of the spin edge states also change (figures 2(c1) and (c2)). We thus can modulate the edge state properties by adjusting the light field.

Then we consider the staggered electric field and exchange field simultaneously (not including the circularly polarized light). These applied external fields lead to an SQAH state with the topological numbers \( (\pm 1, 1/2) \) [10, 15]. The detailed relation of these fields for this SQAH state can be found in the topological phase diagram in our previous work [7]. The SQAH state has a single spin edge state (figures 2(d1) and (d2) for the Chern number case of (1, 1/2); figures 2(f1) and (f2) for the Chern number case of (−1, 1/2)).
Figure 2. Three types of TI edge states and their energy bands. (a1) and (a2) QSH state with Chern number (0, 1); (b1) and (b2) QAH state with Chern numbers (2, 0) ($\chi_2 = -0.15t$); (c1) and (c2) QAH state with Chern numbers (-2, 0) ($\chi_2 = 0.15t$); (d1) and (d2) SQAH state with Chern numbers (1, 1/2) ($\varepsilon_2 = -0.03t, M_{AF} = 0.03t$); (f1) and (f2) SQAH state with Chern numbers (-1, 1/2) ($\varepsilon_2 = 0.03t, M_{AF} = 0.03t$). The red (blue) arrows or bands in the figures denote the spin-up (down) case and the red and blue bands overlap in (a2). The other fixed parameters in all the cases are: the width of ZSiNRs = 16, $\lambda_{so} = 0.03t$.

We can also change the staggered electric fields or exchanged field to modulate the spin polarization and edge state direction. In the following section, we will design different types of the three-terminal TI junctions to study the current behaviors by combining these topological states in different parts of the device.

3.2. The characteristic of ‘nearest path selection’

Now we study the current behavior in the three-terminal topological junction systems. The lead 1 and the conductor are set as the QAH state ($\chi_2 = (2, 0)$) and the output leads (lead 2 and lead 3) are set as the QAH or SQAH state. To show the results more clearly, we only focus on the behavior of spin-up current due to the similarity between the spin-up and spin-down currents. Firstly, we consider that the leads and conductor all are set as QAH states (type 1). Figure 3(a1) shows the cartoon picture of the system. One can see that lead 1 (including the conductor) has a positive spin-up channel in the x-direction (the lower edge), while the output leads have two channels (the lower edges of lead 2 and lead 3). Besides, lead 1 (including the conductor) has a spin-up channel with negative x-direction in the upper edge. Therefore, for the spin-up current incident from lead 1, there exist three possible paths to go through: transmitting to the output leads (lead 2 or lead 3) or be reflected from the conductor. From the transmission spectrum (figure 3(a3)), we find the spin-up current only flows into the lower edge of lead 3, corresponding to a 100% transmittance in a wide range near the Fermi energy. And the local current distribution (figure 3(a2)) near zero energy (at $E = 0.0005$ eV) verifies this transmission result. The reason is that the spin-up edge states have the same direction in lead 3 and conductor, so the spin-up electron can freely pass through lead 3 with a unit transmittance. If we use the right-circularly-polarized off-resonant light instead of the left-circularly-polarized off-resonant light in the lead 3, its topological numbers become ($-2, 0$). Thus, the direction of the edge states in the lead 3 is opposite, which leads to a positive spin-up channel (in the x-direction) in the upper ribbon edge (type 2, figure 3(b1)). In this case, the vertical distance between the spin-up channels (in positive x-direction) of lead 2 and lead 3 is shortened. The local current and transmission results (figures 3(b2) and (b3)) indicate that the current only choose the nearest path in a very small range of the Fermi energy. Then we turn off all spin-up channels of lead 3 by setting it as SQAH state with the Chern number ($-1, 1/2$) (type 3, figure 3(c1)). The results (figures 3(c2) and (c3)) suggest the current transmits from the lower edge of lead 2 in a wide energy range near the Fermi level.

All of the above results clearly show that the spin current prefers the nearest path. However, why does the 100% spin-up transmission in type 2 only present in such a very small range near the Fermi energy? We will discuss the details in section 3.3.
3.3. The characteristic of ‘group-velocity mismatch’

Based on the model of figure 3(b1) (type 2), we further change lead 3 into the SQAH state with the Chern number (1, 1/2) (type 4, figure 4(a)). Through the local current distribution, we find that some spin-up current flow into the lead 2 (figure 4(b)), corresponding to about 30% transmission near the Fermi energy (figure 4(c)). What causes the difference between type 2 and type 4? We can analysis from the energy band. As we know, the slope of bands is proportional to the group velocity. For lead 3 in SQAH state (Chern number (1, 1/2)), it has a small spin-up band slope near $E = 0$, corresponding to the low group velocity (figure 2(d2)). Thus, the larger spin-up band slope in the lead 1 (including the conductor) (figure 2(a2)) results in a significant group-velocity mismatch when spin-up current from lead 1 tries to flow into lead 3. Finally, group-velocity mismatch causes partial spin-up current to be reflected. The reflected spin-up current continues to look for the nearest path and the lower edge channel of the lead 2 is the best choice. Moreover, the transmission from lead 1 to lead 3 increases and arrive about a constant (about 90%) in some larger energy range ($|E| > 0.03$ eV). The reason lies that in that larger energy range, the band slope in lead 3 increases again (figure 2(d2)) and the slope gets close to that of lead 1, which leads to the group-velocity match for each other and a very small reflection between lead 1 and lead 3.

However, we find figure 3(b1) (type 2) also exists the group-velocity mismatch due to the different band slopes between the topological state of (2, 0) and (−2, 0). Why does there is no current flowing into lead 2 near the Fermi energy? From the energy band (figures 2 (b2) and (c2)), one sees that there only exists a small slope difference, causing a very week velocity mismatch. We thus observe that the small velocity mismatch does not affect the transmission (a 100% transmission) in a small energy range near the Fermi level. Out of this small energy range, the decreasing transmission in lead 3 and rising transmission in lead 2
Figure 4. Cartoon pictures ((a), red arrow: spin-up; blue arrow: spin-down), local current distributions ((b), at $E = 0.0005$ eV) and transmission spectra ((c), magenta: spin-up from lead 1 to lead 2; red dotted line: spin-up from lead 1 to lead 3) of type 4. Other fixed parameters are the same as figure 3.

Figure 5. Transmission spectra (upper panel, magenta solid line: spin-up from lead 1 to lead 2; red dotted line: spin-up from lead 1 to lead 3) and local current distributions (lower panel, at $E = 0.0005$ eV) of type 4 with the different light intensity values in lead 3. (a1) and (a2) for $\lambda_\Omega = 0.15t$; (b1) and (b2) for $\lambda_\Omega = 0.25t$; (c1) and (c2) for $\lambda_\Omega = 0.35t$. The fixed parameters are: $\lambda_{1\Omega} = -0.1t$ for lead 1 and lead 2.

The solutions ((3(b3)) are believed to result from this small velocity mismatch. We thus give an explanation of the question raised in section 3.2.

Through the analysis above, based on the model of figure 3(b1) (type 2), we can get a different transmission by adjusting the slope of spin-up bands of leads and conductor. Figure 5 shows the local current distributions, energy bands and transmission spectra with different light intensities. Firstly, in lead 1 (including the conductor) and lead 2, the light intensity $\lambda_\Omega$ is taken a small value (0.1t) simultaneously. Compared to figure 3(b1), the transmission from lead 1 to lead 2 increases from zero to about 20% and transmission from lead 1 to lead 3 decreases from 100% to about 80% for the spin-up current near Fermi energy (figure 5(a1)). And the local current distribution shows the transport details (figure 5(a2)). This is because that the slope difference between lead 1 (including the conductor) and lead 3 is more significant (the illustration of figure 5(a2) for the energy band), corresponding to a stronger velocity mismatch. The large velocity mismatch makes the partial spin-up current from lead 1 to lead 3 being reflected and flowing into lead 2. Moreover, we find the spin-up transmission from lead 1 to lead 2 increases with increasing the light intensity $\lambda_\Omega$ of lead 3 (figures 5(b1), (b2), (c1) and (c2)). Compared with the nearest-path principle, the group-velocity mismatch will dominate when the light intensity applied on lead 3 is large enough. We thus infer that in this case, the velocity-mismatch-induced scattering plays a major mechanics, which makes the current select a secondly-nearest path, rather than the firstly-nearest path.
We call the group-velocity mismatch a scattering engineering in TI transport devices. Thus, one also needs to consider the velocity mismatch in designing spintronic devices based on the TI system.

### 3.4. Spin filter based on the characteristics of TI edge current

We have found that the current has two important features in the transport process: the nearest path principle and group-velocity mismatch. These two characteristics often occur simultaneously during the topological edge current transport. Taking advantage of these characteristics, one can find ways to design spin filters. Here, we take the model of figure 6(a) into account. In this model, the topological state of the conductor (QAH) is different from lead 1 (QSH), by applying the light field in the conductor ($\lambda_\Omega = -0.07t$). The lead 2 and lead 3 are both set as SQAH state ($|E_z| = 0.03t$, $|M_z| = 0.03t$) but with different Chern numbers. Obviously, there exists an adjustable velocity mismatch between the leads and conductor by modulating the light intensity applied to the conductor. From the transmission spectrum (figure 6(d)), there exists asymmetrically positioned transmission peaks around the zero energy for spin-up current. These peaks suggest that there are some resonance transmissions from lead 1 to lead 3. We regard these peaks as the Fano resonance [10]. With the local current distributions (figure 6(g), $E = -0.0086$ eV), we find the cycled current path for resonance. The spin-up current is strongly reflected due to the opposite direction of edge states between the left lead 1 and the conductor, which increases velocity mismatch when spin-up current flows into a conductor from the upper edge of lead 1. Owing to the topological protection, the reflected spin-up current flows downward along the lead 1/conductor boundary to the lower edge. Then it turns rightward in the lower edge and flows upward along the right-lead/conductor boundary to the upper edge. Finally, the cycle-shaped current path occurs (figures 6(g) and (b)). One also notices that there is partial bulk current (not the edge state) flowing near the upper conductor edge from lead 1 to the lead 2. And in the lower conductor edge, there is also a bulk current flowing from the right lead-conductor boundary to the left lead-conductor boundary. To intuitively show this path, we give the cartoon picture for the spin-up case (figure 6(b)). At the same time, the spin-down current flow into lead 3 from lead 1 with almost unit transmittance (figures 6(d), (h) and (c)). Therefore, one can obtain spin-up and spin-down
current from lead 2 and lead 3, respectively. We call this filter a double-output spin filter. Similarly, when the direction of the light field is changed, one can get a double-output spin filter that spin-down current has some resonance transmission from lead 3 (not shown in this paper).

The double-output spin filter can be switched into a single-output spin filter when the light intensity applied on the conductor is enhanced. Figure 6(e) show the spin-up transmission from lead 1 to lead 2 is almost zero (figure 6(i)) near Fermi energy when the light intensity in conductor is taken $-0.15t$. With increasing the light intensity to $-0.35t$ (figure 6(f)), the region of zero transmission has widened near Fermi energy, due to the large velocity mismatch. Therefore, one can obtain only spin-down current from lead 3, which is a single-output spin filter.

4. Conclusion

In summary, we use a combination of different topological junctions to design a serial of three-terminal systems. Based on these TI-junction systems, we have studied the topological edge current behaviors in the transport process. Two important characteristics of current propagation have been found: the nearest-path rule and the velocity-mismatch rule. One can manipulate the topological edge current by utilizing these rules and find some resonance-transportation processes. As an example, we propose a spin filter based on such a three-terminal TI junction with the Fano resonances. And we explain the transmission mechanism by using the local current distribution. We believe this research has very potential usages in the design of 2D-materials-based spintronic devices in the future.

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