Measurable spin-polarized current in two-dimensional topological insulators

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Abstract

We propose a simple method for generating a spin-polarized current in a two-dimensional topological insulator. As z-component magnetic impurities exist on one edge of the Kane–Mele model, a subgap is opened in the corresponding pair of edge states, but another pair of gapless edge states is still protected by the time reversal symmetry. Thus the conductance plateau with the value $e^2/h$ in the subgap corresponds to a single-edge and spin-polarized current. We also find that the spin-polarized current is insensitive to weak non-magnetic disorder. This mechanism for generating spin-polarized currents is independent of the concrete theoretical model and can be generalized to two-dimensional topological insulators, such as HgTe/CdTe quantum wells and silicene nanoribbons.

(Some figures may appear in colour only in the online journal)

1. Introduction

Since graphene, a single-layer honeycomb lattice of carbon atoms, was first prepared in the laboratory by Novoselov et al [1], it has attracted considerable attention due to its novel properties in condensed matter physics and potential applications in devices [2–10]. Graphene is the first independent two-dimensional (2D) crystal to have been experimentally achieved, and it has led to new interest in 2D systems. For example, the Kane–Mele model, a quantum spin Hall effect (QSHE), was first proposed for graphene with spin–orbital coupling, yielding the first example of a topological insulator [11, 12]. Topological insulators are time reversal symmetric systems whose intrinsic spin–orbit coupling (SOC) opens a bulk gap while generating the Kramers doublet of edge states owing to the nontrivial $\mathbb{Z}_2$ invariants of the occupied bands. The edge states force electrons with opposite spin to flow in opposite directions along the edges of the sample, which leads to quantized spin Hall conductance. However, the intrinsic SOC in real graphene is quite weak and the gap opening is small, so the QSHE in graphene is difficult to observe [13]. Nevertheless, recently a monolayer honeycomb lattice of silicon called silicene has been synthesized and it has attracted great attention [14–17]. Silicene has a relatively large intrinsic spin–orbit gap of 1.55 meV, which makes the Kane–Mele type QSHE experimentally accessible [16].

The development of the topological insulator opens up a new and powerful route to spintronic applications due to its spin-dependent edge states. How to generate spin-polarized currents in low-dimensional systems is one of the main challenges in the field of spintronics. The aim of this work is to propose a method for generating a spin-polarized current in a 2D topological insulator. In this paper we theoretically study, as a concrete example, the electronic transport in the Kane–Mele model with magnetic doping on one edge, as shown in figure 1. It should be emphasized that most of the results are also applicable to general 2D topological insulators. Before presenting our detailed calculations, we first analyze why spin-polarized...
current can be generated in the present device. The intrinsic SOC which originates from intra-atomic SOC converts the sample into a topological insulator with a QSHE [11]. The gapless edge states are protected by time reversal symmetry and are thus robust against non-magnetic impurities that do not break this symmetry. However, on the other hand, a pair of edge states is destroyed when magnetic impurities are doped onto this corresponding edge (see figure 1). Because another pair of edge states, with opposite spins containing opposite propagation directions, is still protected by time reversal symmetry, a spin-polarized current in the sample can be observed, which is confirmed by our following calculations.

The rest of the paper is organized as follows. In section 2, we describe the model and give the details of our calculations. In section 3, the numerical results are given. Finally, a brief conclusion is presented in section 4.

2. The model and method

In the tight-binding representation, we consider the Kane–Mele Hamiltonian defined on a honeycomb lattice [11, 12]:

$$H = t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda \sum_{\langle ij \rangle, \sigma} v_i c_{i\sigma}^\dagger x_i c_{j\sigma} + i\alpha \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger (s \times d_i) c_{j\sigma} + \lambda_v \sum_{\langle ij \rangle, \sigma} \xi_{i\sigma} c_{i\sigma}^\dagger c_{j\sigma}. \quad (1)$$

The symbols $\langle ij \rangle$ and $\langle \langle ij \rangle \rangle$ denote the nearest and the next-nearest neighbors, respectively, and $\sigma = \uparrow, \downarrow$ (or $\pm 1$) denotes the spin index. The first term is the nearest neighbor hopping. The second term describes the intrinsic SOC. Here the site-dependent Haldane phase factor [11] $v_{ij}$ is defined as $v_{ij} = (d_1 \times d_2)/|d_1 \times d_2| = \pm 1$, where $d_i$ denotes the vector from one atom to one of its nearest neighbors. $x_i$ is a Pauli matrix describing the electron’s spin. The third term is a nearest neighbor Rashba SOC term, which can be produced by applying an electric field perpendicular to the sheet. The fourth term is a staggered sublattice potential ($\xi_{i\sigma} = \pm 1$). It is interesting to note that equation (1) is almost applicable to silicene except for the Rashba SOC term, which is present for coupling between the nearest neighbors in silicene but for coupling between the nearest neighbors in our model. The focus of this work is on the introduction of magnetic impurities (red square dots in figure 1) on the uppermost zigzag chain of the sample ($n = 1$),

$$H_M = \sum_{i\in \text{nearest } n, \sigma} s_i M c_{i\sigma}^\dagger c_{i\sigma}, \quad (2)$$

where $M$ is the strength of exchange interaction induced by the magnetic impurities. This term breaks the local time reversal symmetry on the upper edge.

The two-terminal conductance of the system can be calculated by the nonequilibrium Green’s function method and using the Landauer–Büttiker formula $G(E) = \frac{e^2}{h} \text{Tr}[\Gamma_L(E)G'(E)\Gamma_R(E)G^\ast(E)]$, where $\Gamma_p(E) = i[\Sigma_p(E) - \Sigma_p^\ast(E)]$ is the linewidth function and $G_p(E) = [G^\ast(E)]^\dagger = 1/[E - \mathbf{H}_{\text{cen}} - \Sigma^\ast - \Sigma_p]$ is the retarded Green function with the Hamiltonian in the center region $\mathbf{H}_{\text{cen}}$ [18]. The self-energy $\Sigma_p$ due to the semi-infinite lead $p$ can be calculated numerically [19].

In order to quantitatively characterize the spin-polarized transport, which is the central topic of this work, we need to calculate, besides the total conductance, the spin-resolved conductance and spin polarization. For a simple and clear definition of polarization, we assume that in the leads the staggered sublattice potential, and the intrinsic and Rashba SOC vanish, and the Hamiltonian of lead $p$ simply adopts the form

$$H_p = t \sum_{\langle \langle ij \rangle \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma}. \quad (3)$$

The spin-resolved conductance matrix is

$$G = \begin{pmatrix} G_{\uparrow\uparrow} & G_{\uparrow\downarrow} \\ G_{\downarrow\uparrow} & G_{\downarrow\downarrow} \end{pmatrix}, \quad (4)$$

which can also be calculated by generalizing the Landauer formula for spin transport. The conductances $G_{\uparrow\uparrow}$ and $G_{\downarrow\downarrow}$ are obtained on the assumption that only spin-up electrons are injected from the left lead into the sample and collected in the right lead. $G_{\uparrow\downarrow}$ and $G_{\downarrow\uparrow}$ can also be calculated in a similar way by assuming that only spin-down electrons are injected from the left lead. The total conductance $G$ and the spin polarization $P$ in lead $R$ can be respectively defined as [20, 21]

$$G = G_{\uparrow\uparrow} + G_{\downarrow\uparrow} + G_{\uparrow\downarrow} + G_{\downarrow\downarrow} \quad (5)$$

and

$$P = \frac{G_{\uparrow\uparrow} + G_{\downarrow\uparrow} - G_{\uparrow\downarrow} - G_{\downarrow\downarrow}}{G_{\uparrow\uparrow} + G_{\downarrow\uparrow} + G_{\uparrow\downarrow} + G_{\downarrow\downarrow}}. \quad (6)$$

Throughout our numerical calculations, the hopping energy $t$ is used as the energy unit. The width $N$ is chosen as $N = 50$ in all calculations and the nearest neighbor atom–atom distance is $a$. The strengths of the intrinsic SOC, the Rashba SOC and the staggered sublattice potential are $\lambda = 0.06t$, $\alpha = 0.05t$, and $\lambda_v = 0.1t$, respectively. These parameters define the system as a 2D topological insulator [11].
3. Numerical results and analysis

First, we investigate the band structures obtained by solving for the band structure of the lattice model in a strip geometry, as shown in figure 2. In the clean case ($M = 0$, figure 2(a)), the edge states traverse the energy gap in pairs. Because the gapless edge states are protected by time reversal symmetry, they are robust against small non-magnetic perturbations [11]. However, in the presence of magnetic impurities ($M \neq 0$, figures 2(b)–(d)) on the upper edge, the corresponding pair of gapless edge states is destroyed and a subgap is opened due to the local time reversal symmetry breaking. Moreover, the magnitude of the subgap opened by the magnetic impurities increases with enhanced $M$, and can reach 0.18 eV for $M = 1$.0$t$. Another pair of gapless edge states, still protected by time reversal symmetry, persists on that edge without magnetic impurities.

Next, we examine the influence of the magnetic impurities on the conductance of the system, as shown in figure 3. In the case of $M = 0$, the quantized conductance plateau appears, with the plateau value $2e^2/h$ coming from the contributions of two pairs of the gapless edge states. For greater values of $M$, the conductance plateau $2e^2/h$ is suppressed and evolves into a conductance plateau $e^2/h$ in the subgap opened by the magnetic impurities. This conductance plateau $e^2/h$ only originates from the gapless edge states on the lower edge without magnetic impurities, which can be seen from figure 4. Without magnetic impurities ($M = 0$), there are two pairs of perfect edge states with opposite spins at the two edges of the sample, so the current through the sample is spin unpolarized. However, when the gapless edge states at the upper edge are destroyed by magnetic impurities ($M \neq 0$), the spin-velocity-locked channels persist only at the lower edge of the sample, with opposite spins moving in opposite directions. For a definite arrangement of bias voltage, there remains only, say, the right-going channel with spin-up electrons. This spin-polarized current is exactly the aim of the present work. Moreover, the spin-polarized current in the sample is really invariant under time reversal.

In the above calculations, magnetic impurities are restricted to just the uppermost zigzag chain of the sample. In fact, we have also numerically tested that, when magnetic impurities reach further inside the upper half of the ribbon, the energy subbands just become slightly complicated, but the above picture of channels is still valid. Therefore, the spin-polarized current can also be induced even if the magnetic impurities reach further inside the upper half of the ribbon.

As introduced earlier, this spin-polarized transport can be investigated in a quantitative way. In figures 5(a) and (b), we show the spin-resolved conductance $G$ and spin polarization $P$ versus the energy $E$ for $M = 1$. In figure 5(a), as expected, the total conductance has only the plateau value $e^2/h$ in the subgap opened by the magnetic impurities. In this energy region, the spin-up electron can fully transport through the sample while the spin-down electron can hardly transport through the sample. We can also find that the spin-up and spin-down electrons are almost unmixed when they transport through the sample, i.e., $G_{\uparrow\downarrow}$ and $G_{\downarrow\uparrow}$ are almost equal to zero. Therefore, in the subgap opened by the magnetic impurities, the spin polarization can even approximate 100% (see figure 5(b)). The plateau $e^2/h$ in the subgap is robust against mismatch scattering between the sample and the leads.
The conductance $G$ versus $E$ for different $M$.

Spin-resolved local density of states (LDOS) along the width of the sample for (a) $M = 0$ and (b) $M = 1$. The energy is chosen as $E = 0.02t$ in the simulation. $N_\sigma = 2n - 1$ and $N_\sigma = 2n$ correspond to the spin-up and spin-down LDOS, respectively, where $N_\sigma = 1, 2, \ldots, 2N$. The black up and down arrows denote spin-up and spin-down carriers. The blue and red curves denote left and right propagation direction.

because of the topological nature of the remaining edge state, while beyond the subgap, the electronic transport will be sensitive to the mismatch between the sample and the leads, so there are resonant tunneling peaks in the conductance beyond the subgap, as shown in figures 3 and 5(a). In this case, the edge states associated with the magnetically doped edge are involved in the transport. But now the backscattering will not be forbidden because of the local time reversal symmetry breaking on this edge. In other words, the incident electrons reaching into the states will be scattered easily by the impurities. The spin-resolved conductances show a resonant tunneling behavior. Therefore, the spin polarization shows strong oscillations in this energy region, as shown in figure 5(b). Furthermore, the oscillations of the spin polarization become stronger and stronger with the strength of the exchange interaction $M$ increasing.

So far, we have seen a single-edge transport with spin polarization in a topological insulator with time reversal symmetry partially broken. A natural question arises: is this spin-polarized transport robust against non-magnetic disorder? To answer this question, we examine the non-magnetic disorder effect on this spin-polarized conductance plateau $e^2/h$. This non-magnetic disorder is simulated by a random on-site potential $w_i$ added for each site $i$ in the sample, where $w_i$ is uniformly distributed in the range $[-w/2, w/2]$. Figures 6(a) and (b) show the conductance $G$ versus the energy $E$ at the disorder strength $w = 0.5t$ and $G$ versus the disorder strength $w$ at the energy $E = 0.02t$, respectively. The results show that the quantum plateau of $e^2/h$ is very robust against non-magnetic disorder...
The conductance $G$ as a function of the energy $E$ for the disorder strengths $w = 0.5t$ (a) and as a function of the disorder strengths $w$ for the energy $E = 0.02t$ (b). The error bars show the standard deviation of the conductance for 100 samples.

Figure 6.

because of the topological origin of the edge state. The quantum plateau maintains its quantized value very well even when $w$ reaches $1.0t$. The robust and stable plateau of $e^2/h$ means that the spin-polarized current of the system is insensitive to weak disorder and protected by time reversal symmetry. In addition, even for a large disorder strength $w$ (e.g., from $w = 1.0t$ to $w = 3.0t$), the conductance increases rather than decreases with the disorder strength increasing. This is because although the strong disorder weakens the edge states, it also results in the mobility of the energy band structure [22], so the value of $G$ increases in the range of $w = 1.0t$ to $w = 3.0t$. With further increasing of the disorder strength, the conductance is gradually reduced to zero and the system eventually enters the insulating regime.

4. Conclusions and discussion

In summary, by partially doping $z$-component magnetic impurities into the Kane–Mele model, we propose a simple mechanism for producing a measurable spin-polarized current in a 2D topological insulator. When magnetic impurities exist on one edge of the sample, the corresponding edge states are destroyed with a subgap opening, but the gapless edge states on the other edge with opposite spin are still protected by time reversal symmetry. Therefore a spin-polarized current with spin-up or spin-down carriers moving in opposite directions can be observed in the system. Moreover, the spin-polarized current is also found to be robust against non-magnetic disorder. A spin-polarized current can be induced provided a pair of edge states on one edge of the sample is destroyed by local time reversal symmetry breaking and another pair is preserved. Therefore, the mechanism for generating spin-polarized currents can be generalized to 2D topological insulators, such as HgTe/CdTe quantum wells and silicene nanoribbons. Similarly, even for three-dimensional topological insulators [23, 24], a spin-polarized current should be induced when only one surface state of the sample is preserved and other surface states are destroyed.

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