Spin-polarized current induced by a local exchange field in a silicene nanoribbon

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Abstract. A mechanism to generate a spin-polarized current in a two-terminal zigzag silicene nanoribbon is predicted. When a weak local exchange field that is parallel to the surface of silicene is applied on one of edges of the silicene nanoribbon, a gap is opened in the corresponding edge states but another pair of gapless edge states with opposite spin are still protected by the time-reversal symmetry. Hence, a spin-polarized current can be induced in the gap opened by the local exchange field in this two-terminal system. What is important is that the spin-polarized current can be obtained even in the absence of Rashba spin–orbit coupling and in the case of the very weak exchange field. That is to say, the mechanism to generate the spin-polarized currents can be easily realized experimentally. We also find that the spin-polarized current is insensitive to weak disorder.

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1. Introduction

The quantum spin Hall effect [1–8], a new quantum state of matter with a nontrivial topological property, is one of the most important topics in condensed matter physics. This novel electronic state has a bulk energy gap separating the valence and conduction bands and a pair of gapless spin-filtered edge states on the sample boundaries. The currents carried by the gapless edge states are immune to nonmagnetic scattering and dissipation due to the protection of time-reversal symmetry. The quantum spin Hall effect was first predicted by Kane and Mele [1] in graphene in which the intrinsic spin–orbit coupling opens a band gap at the Dirac point. However, subsequent works have shown that the intrinsic spin–orbit coupling in graphene is too weak to realize the quantum spin Hall effect under present experimental conditions [9–11].

Recently, a close relative of graphene, a slightly buckled honeycomb geometry of Si atoms called silicene has been synthesized through epitaxial growth [12, 13]. It has been theoretically shown that silicene is a new massless Dirac Fermion system and the strong spin–orbit coupling in silicene may lead to detectable quantum spin Hall effect [7, 14–16]. The possibility of dissipationless spin currents along the edges of silicene and the compatibility of silicene with the silicon-based device make this material particularly attractive for technological applications in spintronics. Very recently, some theoretical studies have proposed that the pure spin current can take place in a quantum spin Hall system with a point contact or magnetic impurities [17, 18]. In this paper, we theoretically study the electron transport through a silicene nanoribbon in the presence of an exchange field on the upper edge of the nanoribbon, as shown in figure 1. The exchange field parallel to the nanoribbon plane may arise due to proximity coupling to a ferromagnet such as depositing Fe atoms to the silicene surface or depositing silicene to a ferromagnetic insulating substrate. Due to the local time-reversal symmetry breaking by the exchange field, an obvious and experimentally observable spin-polarized current can be obtained even for quite weak exchange fields and without Rashba spin–orbit coupling in the system.

2. Model and calculation

In the tight-binding representation, the silicene sample with the exchange field can be described by the following Hamiltonian [15]:

\[
H = -t \sum_{(ij)\alpha} c_{ia}^{\dagger} c_{ja} + \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{(ij)\alpha\beta} v_{ij} c_{ia}^{\dagger} \sigma_{\alpha\beta}^{z} c_{j\beta} - i \frac{2}{3} \lambda_{R} \sum_{(ij)\alpha\beta} \mu_{ij} c_{ia}^{\dagger} \left( \tilde{\sigma} \times d_{0}^{ij} \right)^{z}_{\alpha\beta} c_{j\beta} + M \sum_{i=1}^{10} c_{ia}^{\dagger} \sigma_{i} c_{ia} + \sum_{ia} c_{ia}^{\dagger} \epsilon_{i} c_{ia},
\]

(1)
Figure 1. Schematic diagram of a zigzag silicene nanoribbon with an exchange field (red region) on the upper edge. Silicene consists of a buckled honeycomb lattice of silicon atoms with two sublattices made of A sites (black dots) and B sites (white dots). The green arrow in the red region denotes the direction of the exchange field. The red and blue arrows at the down edges denote propagation directions of the opposite spins in the edge states. The unit cell of the silicene nanoribbon is marked by the dashed lines.

\[ c_{i\alpha}^\dagger \] creates an electron with spin polarization \( \alpha \) at site \( i \); \( \langle ij \rangle \) and \( \langle\langle ij \rangle\rangle \) run over all the nearest and next-nearest neighbor hopping sites, respectively. The first term is the nearest-neighbor hopping with the transfer energy \( t = 1.6 \) eV. For silicene, the intrinsic spin–orbit coupling can be divided into two parts, namely, the effective spin–orbit coupling and the intrinsic Rashba spin–orbit coupling [15]. The intrinsic Rashba spin–orbit coupling is due to the noncoplanar of A and B sublattices in silicene. This is different from that in quantum wells in which the Rashba spin–orbit coupling is due to external inversion asymmetry. The second term describes the effective spin–orbit coupling, where \( \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) is the Pauli matrix of spin and \( \nu_{ij} \) is defined as \( \nu_{ij} = (\vec{d}_i \times \vec{d}_j)/|\vec{d}_i \times \vec{d}_j| = \pm 1 \) with \( \vec{d}_i \) and \( \vec{d}_j \) the two bonds connecting the next-nearest neighbors \( \vec{d}_{ij} \). The third term represents the Rashba spin–orbit coupling, where \( \mu_{ij} = \pm 1 \) for the A (B) site, and \( \vec{d}_{ij}^\theta = \vec{d}_{ij}/|\vec{d}_{ij}| \). The fourth term represents the effect of exchange field with strength \( M \), which breaks the local time-reversal symmetry on the upper edge of the sample. The local exchange field \( M \) may arise due to proximity coupling to a ferromagnet such as depositing Fe atoms to the surface of the upper edge of the silicene nanoribbon or depositing silicene nanoribbon partially to a ferromagnetic insulating substrate.

In the fifth term, \( \varepsilon_i = E_0 + w_i \) is the on-site energy, where \( E_0 \) is the energy of the Dirac point, which is set zero as the energy zero point and \( w_i \) is the on-site disorder energy uniformly distributed in the range \([-w/2, w/2]\) with disorder strength \( w \).

We assume that the temperature is set to zero, and that two clean and semi-infinite silicene ribbons without exchange fields are employed as left and right leads. The two-terminal conductance of the system can be calculated by the nonequilibrium Green’s function method and Landauer–Büttiker formula as

\[
G(E) = \frac{e^2}{h} \text{Tr}[\Gamma_L(E)G^\dagger(E)\Gamma_R(E)G^\dagger(E)],
\]

where \( \Gamma_p(E) = i[\Sigma_p^R(E) - \Sigma_p^L(E)] \) is the linewidth function and \( G^\dagger(E) = [G^\dagger(E)]^\dagger = 1/[E - \mathbf{H}_{cen} - \Sigma_p^L - \Sigma_p^R] \) is the retarded Green function with the Hamiltonian in the center region \( \mathbf{H}_{cen} \) [19]. The self-energy \( \Sigma_p \) due to the semi-infinite lead- \( p \) can be calculated numerically [20].
Figure 2. The conductance $G$ of the zigzag silicene nanoribbon versus $E$ for different $M$. The strength of the Rashba spin–orbit coupling is chosen to be $\lambda_R = 0$.

3. Numerical results and analysis

In the following numerical calculations, we use the hopping energy $t$ as the energy unit. The width of the sample and the strength of the effective spin–orbit coupling are chosen as $N = 50$ and $\lambda_{SO} = 0.3t$ in all calculations, respectively. This effective spin–orbit coupling opens a gap at the Dirac points and establishes the quantum spin Hall effect [15, 21, 22]. In this work, we take the local exchange field $M = 0.1t$, $0.2t$ and $0.3t$. Under this context, the largest exchange field is $M = \lambda_{SO} = 3.9$ meV, which is readily accessible and applicable under current experimental conditions. For instance, by growing the graphene on a ferromagnetic insulator or by adsorbing Fe atoms on top of graphene, the exchange field is about 5 meV [23, 24].

Let us start by describing the influence of the exchange field on the transport properties of the zigzag silicene nanoribbon without disorder, i.e. $w = 0$. In figure 2, the conductance as a function of Fermi energy for different $M$ is studied. In the case of $M = 0$, the conductance $G$ is quantized to a series of plateaus at integers (in the unit of $2e^2/h$) due to the transverse subbands structure of the system with finite width. In the bulk gap, a quantum conductance plateau with the value $2e^2/h$ appears, coming from the contributions of two pairs of gapless edge states. In the presence of exchange field ($M \neq 0$) on the upper edge of the sample, the conductance plateau $2e^2/h$ is suppressed and evolves into a conductance plateau $e^2/h$ in a wide region in the bulk gap. This is because the gapless edge states on the upper edge are destroyed due to the local time-reversal symmetry breaking by the exchange field and the conductance plateau $e^2/h$ is only contributed from the gapless edge states on the lower edge that still protected by time-reversal symmetry and persist on the lower edge of the sample. By diagonalizing the Hamiltonian (1), the subgap opened by the local exchange field is $\pm M$ and the subgap is in the window of the bulk gap. So the conductance is $e^2/h$ when $|E| < M$ only if $E$ is in the bulk gap. Moreover, the range of the quantized conductance plateau $e^2/h$ is extending with increasing in the magnetization $M$. Especially for $M = 0.3t$, the quantized conductance plateau $2e^2/h$ disappear and the quantized conductance plateau $e^2/h$ extends as far as the corresponding region of the bulk gap opened by the effective spin–orbit coupling. When the energy locates...
Figure 3. Calculated energy bands in the zigzag silicene nanoribbon in the presence of the effective spin–orbit coupling for $M = 0$ (a), $M = 0.1t$ (b), $M = 0.2t$ (c) and $M = 0.3t$ (d). The strength of the Rashba spin–orbit coupling is chosen to be $\lambda_R = 0$.

outside of the conductance plateau $e^2/h$, the conductances show slight oscillation between $e^2/h$ and $2e^2/h$ because of the mismatch of interfaces between the leads and the center region.

In order to understand the appearance of the conductance plateau $e^2/h$, we investigate the energy subbands of the silicene nanoribbon for $w = 0$ obtained by solving the lattice model in a strip geometry with open boundary condition in the $y$ direction, as shown in figure 3. The gapless chiral edge states can be clearly seen from the band structure of the pristine silicene ribbons ($M = 0$, figure 3(a)). The gapless edge states are robust against small nonmagnetic perturbations since they are protected by time-reversal symmetry [1]. The electron–hole symmetry is preserved in the gapless edge states, which cross at $ka = \pi$. Since the spin-up and spin-down states are degenerate, the conductance exhibits a series of plateaus in the unit of $2e^2/h$ for the pristine silicene ribbons, as shown in figure 2. When a local exchange field is applied on the upper edge of the silicene nanoribbon, the corresponding pair of gapless edge states is destroyed and a subgap is opened due to the local time-reversal symmetry breaking, as shown in figures 3(b)–(d). Moreover, the magnitude of this subgap opened by the exchange field increases with enhanced $M$, and can be as large as the bulk gap opened by the effective spin–orbit coupling especially for $M = 0.3t$. Another pair of gapless edge states, still protected by time-reversal symmetry, persists on the lower edge of the sample. In the surviving gapless edge states, electrons with opposite spin flow in opposite directions along the lower edges of the sample, which lead to quantized conductance plateau $e^2/h$ and the pure spin current. In other words, there remains only right going channels with spin down working for a definite arrangement of bias voltage in this two-terminal system. It is interesting to notice that the subgap of the upper gapless edge states can be opened even in the absence of the Rashba spin–orbit coupling ($\lambda_R = 0$) when a weak exchange field that is parallel to the surface of the silicene.
nanoribbon is applied at the upper edge of the sample. While the subgap can be opened by a exchange field along the \( z \) direction only when there exists the Rashba spin–orbit coupling in the silicene nanoribbon. In general, a uniform Rashba spin–orbit coupling smaller than the bulk gap does not destroy a quantum spin Hall state [25] unless the screening of the Coulomb interaction is weak and the spatial fluctuation of the Rashba coupling is taken into account [26]. However, the Rashba spin–orbit coupling larger than the bulk gap that destroys the electron spin \( \sigma_z \) conservation tends to destroy the quantum spin Hall effect [2]. The electronic spin \( \sigma_z \) conservation can be directly destroyed by the exchange field that is parallel to the silicene nanoribbon plane, so the subgap can be opened in the absence of the Rashba spin–orbit coupling. These suggest that the spin current can be easily achieved experimentally as the local exchange field is parallel to the surface of the silicene nanoribbon.

To test the above arguments about spin polarization in a more direct way, we study the spin-resolved conductance and spin polarization when the local exchange field is applied on the upper edge of the sample. For the sake of simplicity, we assume that in the leads, the effective and Rashba spin–orbit coupling do not exist, i.e. the Hamiltonian of lead-\( p \) is simply

\[
H_p = -t \sum_{\langle ij \rangle \alpha} c_{i\alpha}^\dagger c_{j\alpha}.
\]

The spin-resolved conductance matrix can be written as

\[
G = \begin{pmatrix} G_{\uparrow \uparrow} & G_{\uparrow \downarrow} \\ G_{\downarrow \uparrow} & G_{\downarrow \downarrow} \end{pmatrix},
\]

which can also be calculated by generalized Landauer formula for spin transport. The conductance \( G_{\uparrow \uparrow} \) and \( G_{\downarrow \downarrow} \) can be obtained when we assume that only spin-up electrons are injected from the left lead into the sample and collected in the right lead. We can also calculate \( G_{\downarrow \uparrow} \) and \( G_{\uparrow \downarrow} \) in the same way by assuming 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 [27, 28]

\[
G = G_{\uparrow \uparrow} + G_{\downarrow \downarrow} + G_{\uparrow \downarrow} + G_{\downarrow \uparrow}
\]

and

\[
P = \frac{G_{\uparrow \uparrow} + G_{\downarrow \downarrow} - G_{\uparrow \downarrow} - G_{\downarrow \uparrow}}{G_{\uparrow \uparrow} + G_{\downarrow \downarrow} + G_{\uparrow \downarrow} + G_{\downarrow \uparrow}}.
\]

Figures 4(a) and (b) show the spin-resolved conductance and spin polarization versus energy \( E \) for \( M = 0.2t \). In figure 4(a), the total conductance manifests itself with the plateau value \( e^2/h \) because the local exchange field is applied on the upper edge of the sample. Due to the topological nature of the edge states, this plateau is insensitive to the mismatch between the sample and the leads. We can also find that the spin-up and spin-down electrons are not mixed when they transport through the sample, i.e. \( G_{\uparrow \downarrow} = G_{\downarrow \uparrow} = 0 \). The spin polarization can almost reach 100% in the subgap opened by the local exchange field (see figure 4(b)) because the spin-down electron can fully transport through the sample while the spin-up electron can hardly transport through the sample in the subgap (see figure 4(a)). Beyond the gap, due to the conduction band mismatch between the central region and the leads, there are resonant tunneling peaks in spin-resolved conductance and spin polarization beyond the subgap induced by the exchange field.
Finally, we examine the effect of the nonmagnetic Anderson disorder on the conductance plateau $e^2/h$ and the spin polarization. The results exhibit that they are quite stable against disorder. Figures 5 and 6 present the effect of disorder on the conductance and the spin polarization, respectively, where the conductance and the spin polarization are averaged over up to 100 random disorder configurations. Figure 5(a) shows the conductance $G$ versus the energy $E$ at different $w$ and $M$, and figure 5(b) shows $G$ versus disorder strength $w$ at different $E$ and $M$. The results show that both of the quantum plateaus of $2e^2/h$ (in the case of $M = 0$) and $e^2/h$ (in the case of $M = 0.2t$) are very robust against nonmagnetic disorder because of the topological origin of the edge states. The quantum plateaus maintain their quantized values very well even when $w$ reaches $2.0t$. When the energy $E$ is in the bulk subbands of the silicene nanoribbon (i.e. $E \approx \pm 0.3t$), the conductance dips appear as $w \neq 0$, as shown in figure 5(a), because the bulk subbands are not protected topologically and are sensitive to the disorder, especially at the edge of the bulk band. Since the plateau of $e^2/h$ is so robust and stable, the spin-polarized current of the system is insensitive to weak disorder and protected by time-reversal symmetry, as shown in figure 6. There is no spin-polarized current in the system when $M = 0$. Disorder can give rise to mobility subgaps in quantum spin Hall systems [29], while spin-dependent mobility subgaps will be induced by disorder in our system due to the presence of the local exchange field. Therefore the polarization curves show dips around $E = 0$ and $0.18t$ in figures 6(a)–(c). From figures 6(d)–(f) we can see that in the case of $w = 0$, the
Current is fully spin polarized as the energy is in the subgaps opened by the local exchange field. For example, $P = 1$ in the case of $E = 0.1t$ for $M = 0.2t$ in figure 6(e). But when the energy is in close vicinity to the margin value of the subband with subgap opened by the local exchange field (i.e. $E = 0.2t$ or $E = 0.25t$ for $M = 0.2t$), the values of the conductance are no longer $e^2/h$ and the current is unpolarized as $w = 0$ (see figure 6(e)) because the edge state destroyed by the exchange field starts to contribute to the conductance. With the increase of the disorder strength $w$, the conductance plateau $e^2/h$ appear, shown as the blue and green lines in figure 5(b), because disorder results in the change of energy band structure [29]. In other words, in this case of parameters ($E = 0.2t$ or $E = 0.25t$ for $M = 0.2t$), the current is unpolarized as $w = 0$, while the spin-polarized current can be induced when the disorder strength $w$ increases, shown as the blue and green lines in figure 6(e). With further increasing of the disorder strength, the conductance gradually reduce to zero and the system eventually enters the insulating regime.

4. Conclusion

In summary, we predict a mechanism to generate a spin-polarized current in a zigzag silicene nanoribbon in the presence of the effective spin–orbit coupling. As a weak exchange field that is parallel to the surface of the silicene is applied on one of the edges of the sample, the corresponding gapless edge state is destroyed and a subgap of the subband is opened even in absence of the Rashba spin–orbit coupling. But another pair of gapless edge states with opposite spin are protected by time-reversal symmetry. Therefore, a spin-polarized current with the spin-up and spin-down carriers moving in opposite directions can be observed in this two-terminal
system. Furthermore, the spin-polarized current is robust against nonmagnetic disorder. The mechanism to generate a spin-polarized current can be easily realized with present technology.

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