Spin current between the two different topological phases in the equilibrium system

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Abstract

In this paper, we analyze the equilibrium spin current in a two-dimensional electron gas with a Rashba spin–orbit coupling at zero bias. Silicene has been successfully synthesized on a two-dimensional honeycomb lattice, and has some unique features due to its buckled structure. By applying the electric and exchange fields, various phases can be realized, such as valley polarized metal (VPM) phase, quantum anomalous Hall state and quantum spin Hall (QSH) state. Both VPM and QSH exhibit metalliclike behavior, we put two different phases in an infinite zigzag nanoribbon, even the weak inhomogeneity of the Rashba medium leads to spin current, and introduce how to control the output polarized current by tuning the electric and exchange fields. Furthermore, we define the concept of bond spin current, and plot the spatial distribution of microscopic spin current. In particular, spin vortex appears when the injected energy is close to the Fermi level, where spin current changes most violently.

1. Introduction

Through many years of efforts, spintronics has emerged as one of the most active areas of physics [1–4], which has been used to store and transfer information [5, 6] controlled by spin current with faster data processing [7, 8] and longer coherent time [9, 10] over the traditional charge-based semiconductor instruments. In recent years, the spintronics research has been made a breakthrough in the following fields. In ferromagnetic metal devices, the manipulating of magnons has been successfully implemented, then the inter-conversion between magnon currents and electron–carried spin and charge currents [2, 8]. The field of antiferromagnetic spintronics can also be discussed from the general perspectives of spin transport, magnetic textures and dynamics, and materials research [4, 11, 12]. Using spin-polarized scanning tunneling microscopy, two distinct stable states have been well separated in a nanostructure comprising an antiferromagnetic chain of Fe atoms. The measurements highlight present experimental capabilities which provides a direct microscopic image of information storage in an antiferromagnet [4].

Nowadays, spin transport becomes a central issue of spintronics. For a long time, physicists have been trying hard to connect spin transport with spin current, and try to give a better understanding of the spin current generation mechanism. Spin Hall effect [13–17] provides a convenient method to produce spin current by an external electric field, which leads to the competition between the Zeeman splitting and spin–orbital (SO) coupling. The electrons with opposite spins will be dejected to opposite directions, an electric current is converted into a spin current perpendicular to the electric field. Spin-momentum locking in the Dirac surface state of a topological insulator [18–21] offers a distinct method for highly efficient charge-to-spin current conversion compared with spin Hall effect in conventional metals. In addition, a temperature gradient applied normal to the Cr O Pt interface induces spin current in Pt, whose magnitude is proportional to magnetization in Cr O [22].

Since the discovery of graphene, more researchers have dedicated to exploit the properties of two-dimensional materials in order to develop faster and low-power electronic devices. The chiral of fermions in graphene can be used for the fabrication of valley electronic devices where one can control the valley flavor of the...
electrons besides its charge. Owing to its small SO coupling \[^{23, 24}\], one can exploit the degree of spin and polarize the output current. Together with the ballistic electronic propagation, graphene can be used to fabricate field-effect transistors, such as \(p-n\) \[^{25}\] and \(p-n-p\) junctions \[^{26}\].

Silicene is a monolayer of silicon atoms arranged in honeycomb lattice \[^{27–30}\], whose band structure is similar to graphene around \(K\) and \(K'\) valleys. Beyond graphene, silicene has a relatively strong SO coupling owing to its buckled structure. The SO coupling could open a gap between the conduction and valence bands. The two inequivalent valleys \(K\) and \(K'\) can be regarded as an additional degree of freedom besides charge and spin, and could be integrated with spin qubit to develop into spin-valley qubit \[^{31}\]. The spin-resolved edge states are split by a perpendicular electric field \(E_z\) and can be tuned by varying its strength. Moreover, the silicene nanoribbons have been synthesized on silver \((110)\) \[^{32}\] and \(\text{MoS}_2\) \[^{33}\] surfaces. Compared with graphene, silicene has a significant advantage in the fabrication of a high-efficiency field-effect spin polarizer \[^{30, 34, 35}\], where the output polarized current can be controlled by both spin and valley. Today, a field-effect silicene transistor has experimentally been realized by transferring silicene on a \(\text{SiO}_2/\text{p}^++\) substrate using a specific growth-transfer-fabrication process at room temperature \[^{36}\].

In order to go further on previous work, we study spin-dependent transport properties of an infinite zigzag silicene nanoribbon in the presence of an electric field. The interplay between the electric and exchange fields leads to the spin asymmetry which is opposite for the two valleys, hence the degree of spin freedom can be tuned by varying \(E_z\). Silicene exhibits plenty of topological phases and Chern numbers can be the modulated by different external fields. There emerges a new type of metal phase in the regions \(E_zM = 0\), the valley-polarized metal (VPM) phase, where the electrons can be moved from a conduction band at valley \(K\) to a valence band at valley \(K'\). In figure 1, we put two different phases together. Then, using the tight-binding Green’s function formalism, it can be shown that the Rashba SO coupling inhomogeneity induces a fully polarized spin current. Spin current flows from one phase where spin is created to another phase where spin is absorbed. Furthermore, we define the bond spin current and evaluate it in terms of spin-resolved equilibrium Green functions, which yield a detailed picture of the charge propagation between two arbitrary sites of the lattice and gives an intuitive explanation of how spin current produces. The above description provides a novel method for generating spin current experimentally due to the Rashba SO coupling inhomogeneity on other crystals.

The remainder of this paper is organized as follows. In section 2, we build up the model Hamiltonian, and define the bond spin current. In section 4, the results of calculation are listed. Section 5 gives a brief summary of this paper.
2. The bond spin current and model

2.1. The bond spin current in the tight-binding model

In order to calculate spin current in real space and plot the spatial profile of the bond spin current, it is advantageous for us to represent the spin-dependent Hamiltonian in the local orbit basis [37–40]

\[ \hat{H}_0 = \sum_{m,\sigma} \varepsilon_m \hat{c}_m \hat{c}_m^\dagger + \sum_{m\neq n,\sigma} t_{mn,\sigma} \hat{c}_m^\dagger \hat{c}_n, \]

where \( \varepsilon_m \) is the onsite energy, and \( t_j \) is the unit 2 × 2 matrix in the spin space. The neighbor hopping \( t_{mn,\sigma}^\dagger = (t_{nm,}\sigma^\dagger \tau^\dagger_\sigma) \) is associated with Rashba SO coupling

\[ t_{mn,\sigma} = \left\{ \begin{array}{l}
- t_{j} - i \lambda_A \hat{\sigma}_x \quad (m = m' + e_x) \\
- t_{j} + i \lambda_A \hat{\sigma}_y \quad (m = m' + e_y).
\end{array} \right. \]

The Heisenberg equation of motion for the local electron number operator \( \hat{N}_m = \sum_{\alpha = \uparrow, \downarrow} \hat{c}_m^\dagger \hat{c}_m \) at site \( m \) follows [41–43]

\[ \frac{d\hat{N}_m}{dt} = \frac{1}{i\hbar} [\hat{N}_m, \hat{H}]. \]

From equation (3), we arrive at the corresponding continuity equation [42, 44]

\[ \dot{\hat{N}}_m = \sum_{j = x, y} (\hat{J}_{m, m + e_j}^\text{e} - \hat{J}_{m - e_j, m}), \]

where \( \hat{J}_{m, m \pm e_j} \) describes the particle flux from site \( m \) to its neighbor site \( m \pm e_j \). The bond spin current \( \hat{J}_{mn,\sigma}^\text{s} = \sum_{\alpha'\sigma'} \hat{J}_{mn,\sigma'}^\text{s} \) is evaluated as the vector sum of different spin-resolved particle current

\[ \hat{J}_{mn,\sigma'}^\text{s} = \frac{e}{i \hbar} (\varepsilon_m^\uparrow \tau^\dagger_\sigma \hat{c}_m^\dagger \hat{c}_n^\dagger \tau_{m\sigma'} - \text{h.c.}), \]

where h.c. stands for the Hermitian conjugate of the first term. The spin-resolved bond spin current describes the outflowing charge current which start as spin \( \sigma \) electrons at the site \( m \) and end up as a spin \( \sigma' \) at the site \( m' \), where possible spin flips are caused by Rashba SO couplings.

The bond spin-current operator for the spin-\( S_x \) component can be defined as the symmetrized product of the spin-\( \frac{1}{2} \) operator \( S_x/2 \) and the bond charge current operator from equation (4) [44]

\[ \hat{J}_{mn,\sigma'}^\text{S_x} \equiv \sum_{\alpha} \frac{1}{4} (\varepsilon_m^\alpha \hat{c}_m^\dagger \hat{c}_n^\dagger \tau_{m\sigma'} - \text{h.c.}), \]

Then, we insert the hopping matrix \( t_{mn,\sigma'} \) in equation (2) into (6), and get the formula for the Rashba SO system

\[ \hat{N}_{mn,\sigma'} = \frac{\lambda_A}{2} \sum_{\alpha} (\varepsilon_{m',\sigma'} \hat{c}_{m',\sigma'}^\dagger \hat{c}_{m,\sigma}^\dagger + \text{h.c.}) + \frac{\lambda_A}{2} \hat{N}_{mn,\sigma'} (\hat{c}_{m,\sigma'} \times (m' - m)) \tau_{m,\sigma'}, \]

where \( \hat{N}_{mn,\sigma'} = \sum_{\alpha, \sigma} (\varepsilon_{m,\sigma'} \hat{c}_{m,\sigma'}^\dagger \hat{c}_{m,\sigma}^\dagger + \text{h.c.}) \) is the bond electron-number operator, which reduces to the standard electron-number operator for \( m' = m \).

These physical quantities are the quantum-statistical average \( \langle \cdots \rangle \) (with respect to a density matrix that has evolved over sufficiently long time so that all interactions are fully established) of the corresponding quantum-mechanical operators in terms of \( \hat{c}_{m,\sigma}^\dagger \) and \( \hat{c}_{m,\sigma} \). This will lead to the expression of \( \langle \hat{c}_{m',\sigma'}^\dagger \hat{c}_{m,\sigma} \rangle \), and defines the lesser Green function \( G_{mn,\sigma,\sigma'}^< \equiv \frac{1}{2} \langle \hat{c}_{m,\sigma}^\dagger \hat{c}_{m',\sigma'} \rangle \), which contains information of the steady-state local transport formalism on the tight-binding model. The decomposition of the bond spin current operator into kinetic and SO terms in equation (7)

\[ \langle \hat{J}^S_{mn}\rangle = \langle \hat{J}^{S_{\text{kin}}}_{mn}\rangle + \langle \hat{J}^{S_{\text{SO}}}_{mn}\rangle \]

leads to a Green function expression for the bond spin current [44–46]

\[ \langle \hat{J}^{S_{\text{kin}}}_{mn}\rangle = \frac{t}{2} \int_{E_{\text{L}}}^{E_{\text{H}}} \frac{dE}{2\pi} \text{Tr} \{ \sigma_3 (G_{mn,\sigma}^< (E) - G_{mn,\sigma}^> (E)) \}, \]

\[ \langle \hat{J}^{S_{\text{SO}}}_{mn}\rangle = (\hat{c}_{m} \times (m' - m)) \frac{\lambda_A}{2} \int_{E_{\text{L}}}^{E_{\text{H}}} \frac{dE}{2\pi} \text{Tr} \{ G_{mn,\sigma}^< (E) + G_{mn,\sigma}^> (E) \}, \]

where \( E_{\text{L}} = -\infty \) and \( E_{\text{H}} = +\infty \).

2.2. The tight-binding model of silicene

The tight-binding Hamiltonian for electrons in silicene considering the electric field and the exchange field has the form
\[
H = -i \sum_{\langle i,j \rangle} \epsilon_{i\alpha} c_{j\alpha} + \frac{\lambda_{SO}}{3} \sum_{\langle i,j \rangle \alpha \beta} \nu_{ij} c_{i\alpha}^{\dagger} \sigma_{\alpha \beta} c_{j\beta} + i \lambda_{R3}(E_{z}) \sum_{\langle i,j \rangle \alpha} c_{i\alpha}^{\dagger} (\sigma \times \hat{d}_{ij}) \gamma_{i\alpha} c_{j\beta}
- \frac{2}{3} \lambda_{R2} \sum_{\langle i,j \rangle \alpha} \mu_{i} c_{i\alpha}^{\dagger} (\sigma \times \hat{d}_{ij}) \gamma_{i\alpha} c_{j\beta} + e\ell E_{z} \sum_{i \alpha} \mu_{i} c_{i\alpha}^{\dagger} c_{i\alpha} + M \sum_{i \alpha} c_{i\alpha}^{\dagger} \sigma_{\alpha} c_{i\alpha},
\]

where \(c_{i\alpha}^{\dagger}\) creates an electron with spin polarization \(\alpha\) at site \(i\), and \(\langle i, j \rangle\) runs over all the nearest/next-nearest neighbor hopping sites. The first term represents the usual nearest-neighbor hopping with the transfer energy \(\epsilon = 1.6\) eV. The second term describes the intrinsic SO coupling with \(\lambda_{SO} = 3.91\) meV. The third and fourth term respectively describes the Rashba SO coupling, in which the third term is linked with the nearest neighbor hopping and its magnitude is proportional to the external electric field \(E_{z}\), \(\lambda_{R3}(E_{z}) = \gamma E_{z}\) with \(\gamma = 10^{-3}\) A\(\text{-}\)eV; the fourth term is linked with the next-nearest neighbor hopping and \(\lambda_{R2} = 0.7\) meV for various topological phases, where \(\mu_{i} = \pm 1\) for the A(B) site, and \(\hat{d}_{ij}\) connecting two sites \(i\) and \(j\). The fifth term describes the staggered sublattice potential, the vertical distance between the A and B sublattices is \(\ell = 0.23\) Å. The sixth term describes the exchange magnetization, the exchange field \(M\) may arise due to the proximity coupling to a ferromagnet by depositing Fe atoms to the silicene surface or depositing silicene to a ferromagnetic insulating substrate.

Following from equation (8), the bond spin current operator in silicene can be decomposed to three terms

\[
\langle \mathbf{J}^{S}_{nm} \rangle = \langle \mathbf{J}^{S\text{(kin)}}_{nm} \rangle + \langle \mathbf{J}^{S\text{(ex)}}_{nm} \rangle + \langle \mathbf{J}^{S\text{(ex)}}_{nm} \rangle,
\]

where the second and third terms describe two different kinds of Rashba SO coupling which contribute to the particle flow.

Following the method of Keldysh [49–51], we use the equation of motion for the Keldysh Green’s function to obtain \(G^{\text{r}}\). Since zero bias is applied in the device, for convenience consideration, we adopt the following formula

\[
G_{mm',\sigma\sigma'}^{n \text{r}} = f(E)(G_{mm',\sigma\sigma'}^{<} - G_{mm',\sigma\sigma'}^{\text{r}(a)}),
\]

where \(f(E)\) is the Fermi–Dirac distribution function, and \(G^{\text{r}(a)}\) is the surface retarded (advanced) Green function taking the boundary conditions into account [35], specific calculations for \(G^{\text{r}(a)}\) is in appendix A.

In the following discussion, we respectively set \(E_{A}\) and \(E_{B}\) in equations (9) and (10) as \(-30\) and \(30\) meV. After these preparations, we obtain spin current \(I_{s}\) by summing the bond spin currents over the longitudinal cross section between the two different phases [44, 45]

\[
I_{s} = \text{Tr} \left( \langle \mathbf{J}^{S\text{(kin)}}_{nn' \text{mm}} \rangle + \langle \mathbf{J}^{S\text{(ex)}}_{nm} \rangle + \langle \mathbf{J}^{S\text{(ex)}}_{nm} \rangle \right).
\]

From equation (10), it is not difficult to find that the Rashba SO contribution to the spin–Sz bond current is zero, so the two terms on the rhs of equation (14) are equal to zero, which simplifies the calculation of spin current in the remainder of this paper. It should be emphasized that the kinetic term can be also influenced by the Rashba SO coupling through \(G^{\text{r}}\).

3. Numerical and discussion

3.1. Topological phases and state density

In this section, we analyze the band structure of a zigzag silicene nanoribbon (figures 3 and B1) and present it in the phase diagram (figure 2). The intrinsic SO coupling \(\lambda_{SO}\) in equation (11) induces a bulk band gap like an normal insulator [47, 52, 53], but protects conducting edge states such as quantum spin Hall effect(QSH) and quantum anomalous Hall effect(QAH).

By applying the staggered potential \(\ell E_{z}\), the spin-resolved band split occurs. This split is valley asymmetric, and has spin inversion symmetry with respect to the boundary of Brillouin zone at \(k = \pi/a\), i.e. \(E^{+}(k) = E^{-}(k)\), where \(a = 38.6\) nm signifies the lattice constant (figure 3; B1). Taking into account only the exchange field, the spin-resolved band split is valley symmetric, spin inversion occurs with respect to \(E = 0\) axis, i.e. \(E^{+}(k) = -E^{-}(k)\) (figure 3; QHS2 and QAH). Let us consider both the electric and exchange fields, the interplay between \(E_{z}\) and \(M\) not only destroys the geometric symmetry of band structure, but also intensifies spin split with \(E^{+}(k) = -E^{-}(k)\) (figure 3; VPM), where the spin–down conduction (spin–up valence) band crosses the Fermi level at \(K(K')\) for \(E_{z} > 0\). Hence, electrons can move from a conduction band at valley \(K\) to a valence band at valley \(K'\), thus we can effectively control spin transport. The results in the phasediagram can be divided to four regions: QSH-region, QAH-region, VPM-region and BI-region (figure 2).

In order to better describe the microscopic spin transport feature, the contour plots of the spin-resolved local density of state (LDOS) of A- and B-atoms near the nanoribbon boundary are shown in figures 4(a)–(d). The LDOS at \(m\) is obtained by calculating the imaginary part of the surface retarded Green’s function:

\[
\rho(E, \mathbf{m}, \sigma) = -\frac{1}{\pi} \text{Im}[G_{\text{mm},\sigma\sigma}(E)] [45].
\]

Figures 4(e)–(g) describe the spin-resolved conductance \(G^{\alpha}\), \(\alpha = \uparrow, \downarrow\) for different phases, which provide us a clear description of the overall nature of transport properties. It should
be emphasized that the sharp peaks of the LDOS (van Hove singularities) occur precisely by the conductance step-jump. The density of states of a 1D periodic structure diverges close to band extrema, thus leads to the pronounced peaks close to the Fermi energy, which is called van Hove singularities. Furthermore, it has been observed in ordered grain boundaries of graphene using scanning tunneling microscopy [54]. The spin-resolved conductance jump height is \(2e^2/h\), the factor 2 is responsible for sublattice pseudospin index. The sizable gap between opposite spin contributions in the quantum conductance results from the band structure asymmetry. In QAH, the Rashba SO coupling \(\lambda_{R2}\) mixes up and down spins, and opens a gap where almost flat modes

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**Figure 2.** All the phases in figure 3 are marked by red hollow circles in the \(E_z - M\) plane. Band gap closes in the phases lying along the dashed lines. Spin Chern number and Chern number are well defined in insulators.

**Figure 3.** The band structure of silicene nanoribbon for various phases. The blue line presents spin-up \(\uparrow\), the red line presents spin-down \(\downarrow\), in QSH1, the energy band is spin degenerate. The vertical axis is the energy in unit of \(t\), and the horizontal axis is the momentum. The Dirac cone represents the bulk spectrum, and the lines linking the Dirac cones are edge states.
appear, thus leads to zero LDOS and a sharp dip of the conductance at zero energy (figure 3 QAH). In QSH2, the sharp peak of LDOS confirms the existence of van Hove singularities, nonzero conductance \( G^I = G^F = e^2/\hbar \) at zero injected energy is caused by the existence of the edge states in the gap (figure 3 QSH2). In VPM2 and BI, the external electric field induces an band gap between electron and hole states which suppresses the transmission of carriers with injected energy \( E_e < E_z \). In figure 4,(a), the width of region without conducting carriers is about \( eE^2z\ell \), which is just the intrasublattice barrier between vertically separated A and B sublattices in the presence of a perpendicular electric field. This agrees well with zero LDOS for both A and B sublattices at zero injected energy (figure 4(d)). In VPM2, by applying the exchange field, there are two regions without carriers corresponding to LDOS (figure 4(c)) and conductance (figure 4(g)) of spin-up and spin-down, respectively, the width of both regions is \( 2e\ell E_z \).

Each topological phase is characterized by the Chern number \( C \) [16, 53], which is well defined when the Fermi level lies in the gap, such as in QAH, QSH2 and BI. It can be calculated by

\[
C = \frac{1}{2\pi} \sum_n \int_{BZ} d^2k \Omega_n(k),
\]

\[
\Omega_n(k) = -2 \sum_{n' = n} \frac{\text{Im} \langle \psi_{nk}\psi_{nk}^\dagger \rangle \langle \psi_{nk}\psi_{nk}^\dagger \rangle}{(\omega_n - \omega_n')^2},
\]

where \( \Omega_n(k) \) is the Berry curvature in the momentum space for the \( n \)th band below the bulk gap, \( \omega_n \equiv E_n/\hbar \), \( \psi_{nk} = \partial H / \partial k_{x,y} \) is the Fermi velocity operator. We numerically diagonalize the Hamiltonian in equation (11) and compute the Berry curvature in figure 5 which is peaked at the corners of the first Brillouin zone. In the phases along the \( M \)-axis in figure 2, the honeycomb lattice preserves the space inversion symmetry for which \( \Omega(k) = -\Omega(-k) \), hence the Berry curvature has the same sign at \( K \) and \( K' \) (figure 5 QAH and QSH2). But in VPM2 and BI, the staggered potential destroys the AB sublattice symmetry, the Berry curvature have opposite signs at \( K \) and \( K' \). In VPM2, the Fermi level does not lie in the gap again, the Chern number is ill-defined.

### 3.2. Spin current in the equilibrium

In order to uncover the underlying physics, the Dirac theory near the Dirac points \( K \) and \( K' \) is employed. We Fourier transform the tight-binding model equation (11) and adopt the low-energy approximation

\[
H_\text{d} = \hbar v_0 (\eta \sigma_z \tau_0 \otimes \tau_z + \eta \sigma_1 \tau_0 \otimes \tau_y) + 4\epsilon E_z \sigma_0 \otimes \tau_z + \lambda \tau_z \tau_0 + \lambda \tau_3 \tau_0 + \lambda \tau_3 (\eta \sigma_y \otimes \tau_x - \sigma_x \otimes \tau_y) / 2,
\]
where $h_1 = \lambda_{SO}\sigma_z + a\lambda_{R2}(k_x\sigma_x - k_y\sigma_y)$, $\tau_a$ stands for the Pauli matrix of pseudospin, $v_F = \frac{\sqrt{2}}{2}$ is the Fermi velocity.

The Hamiltonian $H_T$ can be expressed in matrix form

$$H_T = \begin{pmatrix} E(1, 1) & \hbar v_F k_- & ia\lambda_{R2}k_- & 0 \\ \hbar v_F k_+ & E(1, -1) & -i\lambda_{R1} & -ia\lambda_{R2}k_- \\ -ia\lambda_{R2}k_+ & i\lambda_{R1} & E(-1, 1) & \hbar v_F k_- \\ 0 & ia\lambda_{R2}k_+ & -\hbar v_F k_- & E(-1, -1) \end{pmatrix},$$

its basis is $\Psi^T = (\psi_A, \psi_B, \psi_{A^\dagger}, \psi_{B^\dagger})^T$, where $k_\pm = k_x \pm ik_y$ and the diagonal elements are

$$E(s, \tau_z) = \lambda_{SO}s_z + c'k_z + Ms_z,$$

with the electron spin $s_z = \pm$ and the sublattice pseudospin $\tau_z = \pm 1$.

Along the $M$-axis in the phase diagram (figure 2), the energy spectrum can be gotten by diagonalizing the Hamiltonian $H_T$.

$$E = \pm \sqrt{a^2\lambda_{R2}^2k^2 + (M - s\sqrt{\lambda_{SO}^2 + 2\hbar^2v_F^2k^2})^2}, \approx \pm a\lambda_{R2}k \left(1 + \frac{1}{2} \left(M - s\sqrt{\lambda_{SO}^2 + 2\hbar^2v_F^2k^2} \right) \right)^2,$$

where $s = \pm 1$. When $M = 0$, there are two spin-degenerate Dirac cones for conduction and valence bands with a gap in the bulk spectrum (figure 3 QSH1). As $M$ increases, spin-up (spin-down) Dirac cone is pushed upward (downward). At $M = E_0(E_0 = 1.955\text{ meV})$, QSH2 is realized, the spin-split edge states traverse the gap in pairs (figure 3 QSH2). When $M \leq \lambda_{SO}(1 + a^2\lambda_{R2}^2/\hbar^2v_F^2)$, the band gap can be calculated as $\Delta = |M - s\lambda_{SO}|$. At $M = \lambda_{SO}$, the gap closes. At $M = 4E_0$, QAH is realized where $\lambda_{R2}$ mixes up and down spins, turning the crossing points into the anticrossing points, a gap forms in the bulk spectrum, where only flat modes exist.

In the VPM-region ($E_zM \approx 0$), the energy spectrum reads

$$E = s_zM \pm \sqrt{\hbar^2v_F^2k^2 + (c'k_z - \eta_2\lambda_{SO})^2}, \approx s_zM \pm \frac{c'k_z - \eta_2\lambda_{SO}}{\sqrt{c'^2k_z^2 - \eta_2^2\lambda_{SO}^2}}.$$

when the injected energy $\hbar v_F k_z$ is enough small, the second-order term can be neglected, $E \approx s_zM \pm \frac{c'k_z - \eta_2\lambda_{SO}}{\sqrt{c'^2k_z^2 - \eta_2^2\lambda_{SO}^2}}$.

Both VPM and QSH exhibit metallic-like behavior, we choose an infinite zigzag silicene nanoribbon with $N = 96$ atoms over its longitudinal cross section, then put one VPM phase and one QSH phase together (figure 1). In VPM, the electric field induces another new type of Rashba SO coupling $\lambda_{R1}$, which originates from
the buckled structure. Owing to the Rashba SO coupling inhomogeneity in the device of VPM–QSH, spin is not conserved again, and forced into precession by the effective momentum-dependent magnetic field of SO coupling. Thus spin is pumped from one phase where it is produced to another phase where spin is absorbed. The non-zero spin current through the transverse cross section is due to only the wave functions (or Green functions) near the Fermi level ($T \to 0$), in accord with the general paradigms of the Landau’s Fermi liquid theory where transport quantities are expected to be expressed as the Fermi-surface property, where only weakly quasiparticle excitations are allowed.

We plot the spin current $I_{\uparrow} = I_{\uparrow} - I_{\downarrow}$ as a function of injected energy around the Fermi level (figures 6 and 7), where both the peak and valley values appear. This originates from the band valley asymmetry of spin split in the VPM phase. Below the Fermi level, more spin-up electrons are excited and flow to QSH, $I_{\uparrow} < 0$; above the Fermi level, more spin-down electrons are excited, $I_{\uparrow} > 0$.

Since any eigenstate is spin polarized with $s_z = \pm 1$, the energy interval of spin current can be obtained by solving the eigenequation $H_{\uparrow} \Psi = E\Psi$. For some definite spin $s_z$ in equation (20), the eigenvalues of VPM phase respectively take $E = s_z M \pm \left( e\ell E_z - i\psi \lambda_{SO} \pm \frac{\hbar v_F k^2}{4e\ell E_z - i\psi \lambda_{SO}} \right)$. As $e\ell E_z$ is fixed, the energy interval of spin current depends on the exchange field being $\Delta E = 2M$. When $M$ increases by $E_0$, this interval increases by $2E_0$ (figure 6). A similar conclusion can be drawn in figure 7. As $M$ is fixed, the interval depends on the electric field being $\Delta E = 2e\ell E_z$. When $e\ell E_z$ increases by $E_0$, this interval increases by $2E_0$.

Let us focus on figures 6 and 7, both valley and peak values arrive at the extrema in the device of VPM3 (VPM2)–QSH. This is caused by the special band structure of VPM3 and VPM2, where the conduction band touches with the valence band at $K$ and $K'$, thus VPM3 and VPM2 exhibit better metallic conductive behavior than the other VPM phases. When $M = 2E_0$ as the electric field increases, M–VPM2 is realized at $e\ell E_z = 4\lambda_{SO}$, where a gap appears between the conduction and valence bands (figure 3), which causes the decrease in spin transport capacity in M–VPM2–QSH. When $e\ell E_z = 2E_0$, as the exchange field increases, VPM1 is realized at $M = 4\lambda_{SO}$, where a circle respectively appear at $K$ and $K'$ (figure 3 VPM1), which suppresses the spin transport in VPM2–QSH.

Finally, we put BI and another phase in figure 1, spin current does not generate. This is caused by the special band structure of BI, where the conduction and valence bands are completely separated. Furthermore, we find that, in the devices of SVPM–QSH2(VPM3) and BI–QSH2(VPM3), the spin-up conductance $G^\uparrow$ and spin-down conductance $G^\downarrow$ almost overlap with each other (figure B2).

Figure 6. Spin current of VPM–QSH. In (a) and (b), the staggered potential of VPM is $e\ell E_z = 2E_0$ in (c) and (d), the staggered potential of VPM is $e\ell E_z = 4E_0$. The exchange field of VPM-phase increases from $M = E_0$ to $M = 6E_0$. 

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3.3. The effect of width on the spin current

We change the nanoribbon width from \(N = 48\)–\(96\). In the device of VPM–QSH, the spin current curves with different widths presents a slight separation only in a small interval around the extrema (figures B3 and 8). As \(N\) increases, spin current tends to a fixed value. In figures 9\((a)\) and \(9(c)\), the device consists of two phases which own the same exchange field, the spin current curves of M–VPM3 and QAH–VPM1 with different widths nearly overlap with each other. This can be attributed to the similarity of band structure between the two phases. Next, we choose two VPM phases with the same exchange field, we can draw similar conclusions, small separation only appears around the extrema in the devices of VPM3–M–VPM2 (figure 9\((b)\)) and VPM1–VPM2 (figure 9\((d)\)). In the devices of M–M–VPM2 and QAH–VPM2, we get the same conclusion, we do not all of them here.

3.4. The bond spin current

We have analyzed the physical meaning of equilibrium spin current in the weakly inhomogenous Rashba medium (a 2D electron gas with a Rashba spin–orbit interaction). Here, we relate these currents with real spin transport. Spin current transfers spin from areas where it is produced to areas where spin is absorbed. To better investigate mesoscopic features of such equilibrium spin current, we employ the concept of bond spin current of Rashba SO coupled system to describe spin transport between two arbitrary sites on the lattice model, and give an intuitive understanding of spin current generation. The local spin current \(I_{\text{m}}\) describes spin-resolved particle current at site \(m\) which can be viewed as the vector sum of particle current \(J_{\text{m}} = \sum_{m'\neq m} \langle J_{\text{m}m'}^{\text{kin}} \rangle\).

In figure 1, the device consists of two phases, we respectively choose ten columns for each phase and plot the spatial distribution of local spin current. In figure 10, VPM3 lies in the left area of dashed line, and QSH1 lies in the right area. In figures 6 and 7, spin current is equal to zero when the injected energy is far away from Dirac points \(K\) and \(K'\), and the corresponding local spin current profile is fixed. In figures 10\((a)\) and \(10(f)\), we choose the injected energy of \(E = \pm 20\) meV and respectively plot the local spin current profiles. In the nontopological area of VPM3, the edge states and bulk state coexist, no matter the injected energy is positive or negative, the local spin current on the boundary always flow in the same direction. But in the interior of ZGNR, the local spin current direction reverses with incident energy changing from negative to positive. This phenomenon can be explained by the fact that the spin split of VPM3 is band valley asymmetric in figure 3, where at \(K\), the spin–up Dirac cone crosses the Fermi level; at \(K'\), the spin–down Dirac cone crosses the Fermi level. At \(E = -20\) meV, in the VPM3 area, the magnitude of the local current flowing on the lower boundary is much larger than that on the
upper boundary (figure 10(a)); at $E = 20$ meV, the result is just the opposite (figure 10(f)). In the QSH1 area, the local spin current on the boundary always flows in the same direction, which coincides with band valley symmetry of QSH1 (figure 3). Here, the corresponding spin Hall accumulation deposited by spin current on the lateral boundaries in different phases is caused by the SO force in equation (11).
From figures 6 and 7, we know that spin current varies most dramatically near the Fermi level, meanwhile spin vortex begin to appear. At $E = \pm 5$ meV, only a small number of spin vortices appear in the VPM3 area (figures 10(b) and (c)); but at $E = \pm 3$ meV, the whole device is nearly covered with spin vortex (figures 10(c) and (d)). These vortices, like pumps, carry electrons with different spins from one place to another. The vortex

\[ \text{Figure 10. The spatial profiles of the local spin current in the device of VPM3\textendash}QSH1 at } E = \pm 20, \pm 5, \pm 3 \text{ meV in (a)-(f), VPM3 (QSH1) lies in the left (right) area of dashed line, the length of the arrow is proportional to the magnitude of the local spin current.} \]
pattern is caused by the Rashba SO coupling inhomogeneity, and becomes the sign of the speed of spin current change. Through the local spin current profiles, we construct the basic physical understanding about spin transport between two sites. We can also find spin vortex in the other devices, the local spin current profiles of VPM4–QSH1 are plotted in figures B4(a) and (b), VPM3–QSH2 in figures B4(c) and (d), VPM4–QSH2 in figures B4(e) and (f).

4. Conclusion

In conclusion, we have provided a novel method to equilibrium spin current generation due to the Rashba SO coupling inhomogeneity in a two-dimensional gas, and introduce how the output polarized current is controlled by tuning the electric and exchange fields in detail. In silicene, we apply the electric and exchange fields, various phases can be realized, such as VPM, QSH1 and QAH. In the VPM phase, the spin split is band valley asymmetric with \( E^+(k) = -E^-(k) \), which is precisely accompanied by the asymmetrical distribution of LDOS. Next, the ZGNR width effect is investigated, spin current only presents a slight change near the extrema. Furthermore, we employ the concept of the bond spin current to describe spin current along a single bond between two atoms of a two-dimensional honeycomb lattice model of an SO coupled system, and calculate it in terms of equilibrium Green functions. Using the bond spin current, we build a correspondence between local spin current profile and band structure, and explicitly explains how spin current is pumped from one phase to another. In particular, we find spin vortex, and it becomes a sign of how fast spin current changes. This work highlights our further research, we will try to realize spin current in more complex materials by utilizing Rashba SO coupling inhomogeneity.

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Appendix A. Basic formulas

A.1. The continuity equation

We can apply the familiar continuation equation in the quantum mechanics

\[
\frac{\partial\rho}{\partial t} + \nabla \cdot \mathbf{j} = 0
\]  

(A.1)

to the SO coupled system, with charge density \( \rho = e|\Psi(\mathbf{r})|^2 \) and the charge current density \( \mathbf{j} = e\text{ Re}[\Psi(\mathbf{r})\Psi^*(\mathbf{r})] \). Following from the definition of the classical charge current density \( \mathbf{j} = en(\mathbf{r})\mathbf{v} \) with \( n(\mathbf{r}) \) the particle density, its quantized form can be written as follows

\[
\mathbf{j} = e\mathbf{n}(\mathbf{r})\mathbf{v} + \frac{\mathbf{\mathbf{\hat{v}}(\mathbf{r})} + \mathbf{\mathbf{\hat{v}(\mathbf{r})}}}{2},
\]  

(A.2)

which is symmetrized to ensure that it is a Hermitian operator [44, 55]. In the two-dimensional Rashba medium

\[
\hat{\mathcal{H}} = \frac{\hat{\mathbf{P}}^2}{2m^*} + \frac{\lambda_y}{\hbar}(\hat{p}_y\mathbf{\hat{e}}_x - \hat{p}_x\mathbf{\hat{e}}_y) + V_{\text{conf}}(x, y),
\]  

(A.3)

where \( m^* \) is the effective mass and \( V_{\text{conf}}(x, y) \) is the confined potential. The velocity operator \( \mathbf{\hat{v}} = \frac{1}{i\hbar}[\hat{\mathbf{r}}, \hat{\mathcal{H}}] \) should be modified owing to the presence of Rashba SO coupling

\[
\mathbf{\hat{v}} = \frac{\mathbf{\mathbf{\hat{P}}}}{m^*} - \frac{\lambda_y}{\hbar}(\hat{\mathbf{e}}_y\mathbf{\hat{e}}_x - \hat{\mathbf{e}}_x\mathbf{\hat{e}}_y),
\]  

(A.4)

where \( \mathbf{\mathbf{\hat{e}}}_x \) and \( \mathbf{\mathbf{\hat{e}}}_y \) respectively describe the unit vectors along the x and the y-axis.
The analogous continuity equation of the spin density \( \rho_s^i \) is

\[
\frac{\partial \rho_s^i}{\partial t} + \nabla \cdot \mathbf{J}^s = S_s^i,
\]

(A.5)

with the spin current density

\[
\mathbf{J}^s = \frac{\hbar}{2} \Psi^\dagger(r) \sigma^i \hat{v} \Psi(r) + \frac{\hbar}{2} \sigma^i \hat{v} \Psi^\dagger(r) \Psi(r)
\]

(A.6)

and a non-zero spin source

\[
S_s^i = \frac{\hbar}{2} \text{Re} \left( \Psi^\dagger(r) \frac{i}{\hbar} [\hat{H}, \sigma^i] \Psi(r) \right).
\]

(A.7)

The non-zero \( S_s^i \neq 0 \) term leads to non-conservation of spin in the presence of Rashba SO couplings. Then, we can define the Hermitian operator of the spin current density

\[
\mathbf{J}_k^s = \frac{\hbar}{2} \sigma^i \hat{v}_k + \hat{v}_k \sigma^i,
\]

(A.8)

which is a tensor with nine components.

### A.2. Green function

In what follows we show how to calculate the retarded surface Green’s function \([34, 43, 56, 57]\) of the left (right) lead \( G_L = g_{00}^L (G_R = g_{M+1,M+1}^R) \)

\[
g_{00}^L = [(E + i\eta) \mathbf{I} - H_{00} - H_{00}^\dagger \hat{T}]^{-1},
\]

(A.9)

\[
g_{M+1,M+1}^R = [(E + i\eta) \mathbf{I} - H_{M+1,M+1} - H_{M+1,M+1}^\dagger \hat{T}]^{-1},
\]

(A.10)

where \( \mathbf{I} \) is the identity matrix, the role of \( i\eta \) can make poles of the Green’s functions off the real axis and leads to a retarded response. \( H_{00}(H_{M+1,M+1}) \) is the Hamiltonian of a unit cell in the left (right) lead, and \( H_{00}(H_{M+1,M+1}) \) describes the coupling between two two neighbor unit cells in the left (right) lead.

The transformation matrices \( T \) and \( \tilde{T} \) are calculated from the Hamiltonian matrix elements via iterative algorithm. We begin with \( t_0, \tilde{t}_0 \)

\[
t_0 = [(E + i\eta) \mathbf{I} - H_{00}]^{-1} H_{00},
\]

(A.11)

\[
\tilde{t}_0 = [(E + i\eta) \mathbf{I} - H_{00}]^{-1} H_{00}.
\]

(A.12)

Then, we employ the recursion method to calculate \( t_i \) and \( \tilde{t}_i \)

\[
t_i = (\mathbf{I} - t_{i-1} \tilde{t}_{i-1} - \tilde{t}_{i-1} t_{i-1})^{-1} t_{i-1}^2,
\]

(A.13)

\[
\tilde{t}_i = (\mathbf{I} - t_{i-1} \tilde{t}_{i-1} - \tilde{t}_{i-1} t_{i-1})^{-1} \tilde{t}_{i-1}^2.
\]

(A.14)

We repeat this step until \( t_m, \tilde{t}_m < \varepsilon \), as small as one wishes. This method provides a rapid convergence, which considers a large set of \( 2^l \) unit cells after \( \ell \) iterations. The transfer matrices \( T \) and \( \tilde{T} \) can be calculated using the following expansion

\[
T = t_0 + \tilde{t}_0 t_1 + \tilde{t}_0 \tilde{t}_1 t_2 + \cdots + \tilde{t}_0 \tilde{t}_1 \cdots t_{m}.
\]

(A.15)

\[
\tilde{T} = \tilde{t}_0 + t_0 \tilde{t}_1 + t_0 \tilde{t}_1 t_2 + \cdots + t_0 t_1 \cdots \tilde{t}_m.
\]

(A.16)

Next, we merge the device with the right lead layer by layer from \( l = M \) to \( l = 2 \), the new surface Green functions are found by the following recursion formula

\[
g_{ll}^R = [(E + i\eta) \mathbf{I} - H_{ll} - H_{ll}^\dagger \Psi^\dagger_{l+1,l+1} H_{l+1,l+1}^\dagger]^{-1}.
\]

(A.17)
Finally, the total Green function $G' = g_{i1}$ can be calculated

$$g_{i1} = [(E + i\eta)I - H_{i1} - \Sigma_L - \Sigma_R]^{-1},$$  \hspace{1cm} (A.18)

which takes the interaction between the device and left (right) lead through the retarded self-energy $\Sigma_L(\Sigma_R)$

$$\Sigma_L = H_{01}g^L_{0\alpha}H_{01},$$  \hspace{1cm} (A.19)

$$\Sigma_R = H_{21}g^R_{2\alpha}H_{21},$$  \hspace{1cm} (A.20)

The coupling function between the device and left (right) lead is defined as

$$\Gamma_L = i(\Sigma_L - \Sigma_L^\dagger),$$  \hspace{1cm} (A.21)

$$\Gamma_R = i(\Sigma_R - \Sigma_R^\dagger).$$  \hspace{1cm} (A.22)

In view of the presence of the staggered potential $E_z$ and exchange field $M$ in equation (11), the Green’s function can be decomposed into two block-diagonal parts: spin-up and spin-down. The conductance $G$ of the nanoribbon is spin-resolved [34, 50]

$$g_{i1} = \begin{pmatrix} g^\uparrow_{i1} & 0 \\ 0 & g^\downarrow_{i1} \end{pmatrix},$$  \hspace{1cm} (A.23)

Therefore, the transmission probability follows by

$$T^\alpha(E) = \text{Tr}[\Gamma_L g^\alpha_{L1} \Gamma_R g^\alpha_{R1}], \quad (\alpha = \uparrow, \downarrow),$$  \hspace{1cm} (A.24)

where $\alpha$ is the spin index. We employ the Landauer formula to calculate the spin-resolved conductance

$$G^\alpha = \frac{2e^2}{h} T^\alpha(E), \quad (\alpha = \uparrow, \downarrow).$$  \hspace{1cm} (A.25)

So the total conductance through the silicene ribbon is

$$G = G^\uparrow + G^\downarrow.$$  \hspace{1cm} (A.26)

### Appendix B. Spin current and band structure

In figure B1, we respectively plot the band structure of M-phase, SVPM-phase and M–VPM1-phase. Figure B2 describes the spin-resolved conductance of VPM2–QSH, SVPM–QSH and BI–QSH. Figure B3 describes how the ZGNR width affects spin current, it only presents a slight change around the extremum. Figure B4 describes the local current distribution at $E = \pm 5$ meV where VPM phase lies in the left area of dashed line and QSH lies in the right area of dashed line. It is not difficult to find that a large number of spin vortexes appear, especially in the QSH area.

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**Figure B1.** The band structure of M, SVPM and M–VPM1 phases.
Figure B3. Spin current of VPM–QSH1. The width of the nanoribbon changes from $N = 32$ to $N = 56$. 

Figure B2. The spin-resolved conductance of VPM2–QSH, SVPM–QSH and BI–QSH.
Figure B4. The spatial profiles of the local spin current in the device of VPM–QSH at $E = \pm 5$ meV. VPM (QSH) lies in the left (right) area of dashed line, the length of the arrow is proportional to the magnitude of the local spin current.

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