Controllable intrinsic DC spin/valley Hall conductivity in ferromagnetic silicene: Exploring a fully spin/valley polarized transport

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Abstract

We study intrinsic DC spin and valley Hall conductivity in doped ferromagnetic silicene in the presence of an electric field applied perpendicular to silicene sheet. By calculating its energy spectrum and wavefunction and by making use of Kubo formalism, we obtain a general relation for the transverse Hall conductivity which can be used to obtain spin- and valley-Hall conductivity. Our results, in the zero limit of the exchange field, reduces to the previous results. Furthermore we discuss electrically tunable spin and valley polarized

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transport in ferromagnetic silicene and obtain the necessary conditions for observing a fully spin or valley polarized transport.

Keywords: A. Ferromagnetic silicene; D. Tight-binding model; D. spin/valley Hall conductivity; D. Fully spin/valley polarized transport.

1 Introduction

Since successful isolation of a single layer of graphite\cite{1}, graphene, as the first real two-dimensional lattice structure which shows novel appealing properties\cite{2, 3}, many researchers try to synthesis or isolate new two-dimensional materials. These efforts result in finding other two-dimensional materials such as BN\cite{1}, transition metal dichalcogenides (TMDs)\cite{5} and recently a monolayer of silicon, known as silicene\cite{6, 7, 8, 9}.

Silicene is a monolayer of silicon atoms arranged in a honeycomb lattice structure as similar as graphene. While, as in graphene, its low-energy dynamics near the two valleys at the corner of the hexagonal Brillouin zone is described by the Dirac theory, its Dirac electrons, due to a large spin-orbit (SO) interaction, are massive with a energy gap as $1.55\text{meV}$\cite{10, 11}. Furthermore, due to the large ionic radius, silicene is buckled\cite{10} such that the A and B sublattices of honeycomb lattice shifted vertically with respect to each other and sit in two parallel planes with a separation of $0.46\text{nm}$\cite{11, 12}. The buckled structure of silicene allows to tune its band gap via an electric filed applied perpendicular to its layer. These features donate many attractive properties to silicene\cite{11, 13, 14, 15, 16, 17, 18, 19, 20}.

The SO interaction in silicene is strong, so it is a suitable candidate to study the spin-based effects. Due to this fact, recently silicene has been the subject of strong interest\cite{21, 22, 23, 24}. 


In addition to the spin degree of freedom which is the footstone of the spintronics, the valley degree of freedom in silicene, as in graphene\cite{26, 27, 28}, and MoS$_2$\cite{29, 30, 31, 32}, can be manipulated and hired in a new technology known as valleytronics. One can populate states preferentially in one valley to achieve valley polarization. One way is to use circular polarized light which was discussed theoretically\cite{29}. Another way is to apply a vertical external magnetic field to silicene sheet, so Landau levels form in the electronic density of states. Then, if an excitonic gap via an external vertical voltage included, $n = 0$ Landau level splits into distinct valley- and spin-polarized levels\cite{19}. This is in contrast to that occurs in graphene, in which $n = 0$ Landau level only splits between two distinct valley-polarized spin degenerated energy levels\cite{33, 34, 35, 36}. In other way, as in graphene\cite{37, 38}, the spin/valley polarized current is obtained in silicene\cite{39} junctions by deposing a ferromagnet on the top of its surface. These features make silicene a promising candidate for spin- and valleytronic technology.

In this paper, we consider DC valley/spin Hall conductivity in a ferromagnetic silicene (a silicene sheet with ferromagnet deposed on the top of its surface). We obtain a general relation for its transverse Hall conductivity which can be use to calculate spin/valley Hall conductivity and to discuss possible phase transitions. Furthermore, we obtain the conditions necessary to realize fully valley/spin polarized transport, which depends on the doping, exchange magnetization and the applied perpendicular electric field. The paper is organized as follows. Sec.II is devoted to introduce the Hamiltonian model and obtain the general relation for the transverse Hall conductivity. In Sec.III we present our results and discussion. Finally in Sec.IV we end this paper by summary and conclusions.
2 Model Hamiltonian

The low-energy dynamic in a ferromagnetic silicene, subjected to a uniform electric field applied perpendicular to silicene’s plane, is given by [10, 39]

\[
H_{\eta,s_z} = \hbar v_F(k_x \tau_x - \eta k_y \tau_y) - \eta s_z \Delta_{so} \tau_z + \Delta_z \tau_z - s_z M, \tag{1}
\]

which acts in the sublattice pseudospin space with a wavefunction as \(\Psi_{\eta,s_z} = \{\psi_{\eta,s_z}^A, \psi_{\eta,s_z}^B\}^T\).

The first part of the Hamiltonian is the Dirac hamiltonian describing the low-energy excitations around Dirac points (\(\mathbf{K}\) and \(\mathbf{K}'\) denoted by \(\eta\) index) at the corners of the hexagonal first Brillouin zone. This term arises from nearest neighbor energy transfer. \(v_F = \) is the Fermi velocity of silicene, \(\tau_i (i = x, y, z)\) are the Pauli matrixes and \(\mathbf{k} = (k_x, k_y)\) is the two dimensional momentum measured from Dirac points. The second term is the Kane-Mele term for the intrinsic spin-orbit coupling, where \(\Delta_{so} = 3.9meV\) [10] denotes to the spin-orbit coupling and \(s_z\) index referred to two spin degrees of freedom, up \((s_z = +)\) and down \((s_z = -)\). The third term is the on-site potential difference between \(A\) and \(B\) sublattice, arising from the buckled structure of silicene when a perpendicular electric field is applied with \(\Delta_z = E_z d\) where \(E_z\) is the electric field and the \(2d = 0.46nm\) is the vertical separation of two different sublattice’s plane. The last term is the exchange magnetization where \(M\) is the exchange field. The exchange field my be due to proximity effect arising from a magnetic adatom deposed on the surface of the silicene [10] or from a magnetic insulator substrate like \(EuO\) as proposed for graphene [37].

We obtain the energy spectrum, by diagonalizing the Hamiltonian matrix given in Eq.(1), as

\[
\epsilon_{\nu}^{\eta,s_z} = \nu \sqrt{\Delta_{\eta,s_z}^2 + (\hbar v_F k)^2} - s_z M, \tag{2}
\]

4
where $\nu = + (\nu = -)$ denotes the conduction (valance) bands, $\Delta_{\eta,s_z} = \eta s_z \Delta_{so} - \Delta_z$ and $k = \sqrt{k_x^2 + k_y^2}$. The corresponding wavefunctions are given by

$$
\Psi_{\eta,s_z}^{\nu}(k) = \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{2\chi_{\eta,s_z}}}
\begin{pmatrix}
\sqrt{\chi_{\eta,s_z} - \nu \Delta_{\eta,s_z}} \\
\nu \sqrt{\chi_{\eta,s_z} + \nu \Delta_{\eta,s_z}} e^{-i\eta \phi_k}
\end{pmatrix},
$$

where $\chi_{\eta,s_z} = \sqrt{\Delta_{\eta,s_z}^2 + (\hbar v_F k)^2}$ and $\phi_k = \tan^{-1}(k_y/k_x)$. Figure 1 shows the energy spectrum of silicene (Fig. 1(a)) and ferromagnetic silicene with $M = \Delta_{so}/2$ for three different values of the electric field, $\Delta_z = 0$ plotted in Fig. 1(b), $\Delta_z = \Delta_{so}$ in Fig. 1(c) and $\Delta_z = 2\Delta_{so}$ in Fig. 1(d). These figures show the energy spectrum around $K$. The energy spectrum around $K'$ for zero electrical potential, $\Delta_z = 0$, is equal to that of $K$ point. To obtain the other energy-spectrum plots it is enough to reflect the energy-band plots with respect to $E = 0$ and exchange spin up and down.

DC transverse Hall conductivity, $\sigma_{xy}$, written in the Kubo formalism, is given by

$$
\sigma_{xy}^{\eta,s_z} = -\frac{e^2}{A} \sum_k \frac{f(\varepsilon_{+}^{\eta,s_z}) - f(\varepsilon_{-}^{\eta,s_z})}{(\varepsilon_{+}^{\eta,s_z} - \varepsilon_{-}^{\eta,s_z})^2}
\times \langle \Psi_{-}^{\eta,s_z} | v_y | \Psi_{+}^{\eta,s_z} \rangle \langle \Psi_{+}^{\eta,s_z} | v_x | \Psi_{-}^{\eta,s_z} \rangle,
$$

where $A$ is the area of the sample and velocity components can be obtained from the Hamiltonian and using relation $v_{ki} = \frac{1}{\hbar} \frac{\partial H}{\partial k_i}$. Furthermore $f(\varepsilon_{+}^{\eta,s_z}) = 1/(1 + e^{\beta(\varepsilon_{+}^{\eta,s_z} - \mu)})$ is Fermi-Dirac distribution function with $\mu$ being the chemical potential which at zero temperature is equal to Fermi energy. After calculating the expectation values of the velocities from Eq. 3 and substituting them in Eq. 4 we get

$$
\sigma_{xy}^{\eta,s_z} = \frac{\eta e^2 v_F^2 \hbar}{8 \pi} \int kdk \frac{\Delta_{\eta,s_z}}{\chi_{\eta,s_z}^3} (f(\varepsilon_{+}^{\eta,s_z}) - f(\varepsilon_{-}^{\eta,s_z})).
$$

We restrict our consideration to zero temperature. So we can solve this equation analytically and obtain a general relation for $\sigma_{xy}^{\eta,s_z}$ for all arbitrary values of exchange field, $M$, and Fermi
energy, \( \mu \) which is

\[
\sigma_{xy}^{\eta,s_z} = -\eta \frac{e^2}{4\pi\hbar} \text{sgn}(\Delta_{\eta,s_z}),
\]

(6)

when \(|\mu + s_z M| < |\Delta_{\eta,s_z}|\) and

\[
\sigma_{xy}^{\eta,s_z} = -\eta \frac{e^2}{4\pi\hbar} \frac{\Delta_{\eta,s_z}}{|\mu + s_z M|},
\]

(7)

when \(|\mu + s_z M| > |\Delta_{\eta,s_z}|\). These equations are the main result of this paper. Here \text{sgn}(x)\) is sign function which is 1 for \(x > 0\), 0 for \(x = 0\) and -1 for \(x < 0\). The conditions \(|\mu + s_z M| < |\Delta_{\eta,s_z}|\) and \(|\mu + s_z M| > |\Delta_{\eta,s_z}|\) determine boundaries which separate different phase states. This can be examined by calculating the spin- and valley-Hall conductivity which are defined\cite{42, 43, 44, 45} as

\[
\sigma_{xy}^s = \frac{\hbar}{2e} \sum_{\eta,s_z} s_z \sigma_{xy}^{\eta,s_z},
\]

and

\[
\sigma_{xy}^v = \frac{1}{2e} \sum_{\eta,s_z} \eta \sigma_{xy}^{\eta,s_z},
\]

respectively. This will be explained further in the next section where we present our results.

3 Results and discussions

In this section we present our results. First we examine our general result in the zero limit of \(M\) and \(\mu\). When \(M = 0\) and \(\mu = 0\), only \(|\mu + s_z M| < |\Delta_{\eta,s_z}|\) is satisfied, so we have

\[
\sigma_{xy}^{\eta,s_z} = -\eta \frac{e^2}{2\hbar} \text{sgn}(\Delta_{\eta,s_z}).
\]

This yields

\[
\sigma_{xy}^s = -\frac{e}{4\pi} [\text{sgn}(\Delta_{+,+}) - \text{sgn}(\Delta_{+,-})],
\]

(8)

\[
\sigma_{xy}^v = -\frac{e}{4\pi\hbar} [\text{sgn}(\Delta_{+,+}) + \text{sgn}(\Delta_{+,-})],
\]

(9)

for DC spin- and valley-Hall conductivity of a silicene sheet, if an electric field applied perpendicular to its plane. When \(0 \leq |\Delta_z| < \Delta_{so}\) these equations yield \(\sigma_{xy}^s = -\frac{e}{2\pi}\) and \(\sigma_{xy}^v = 0\),
indicating an intrinsic quantized spin Hall conductivity beside a zero valley Hall conductivity. This regime, as mentioned in previous works\cite{14, 21}, corresponds to a topological insulating (TI) phase characterized by a quantized nonzero spin-Hall conductivity which arises from the presence of gapless helical edge mode. When $|\Delta_z|$ becomes equal to $\Delta_{so}$, we have $\sigma_{xy}^s = -\frac{e}{4\pi}$ and $\sigma_{xy}^v = -\frac{e}{4\pi\hbar}$. In this regime silicene is a spin valley polarized metal (SVPM). If the electric filed increases further such that $\Delta_{so} < |\Delta_z|$, the spin and valley Hall conductivity become $\sigma_{xy}^s = 0$ and $\sigma_{xy}^v = -\frac{e}{2\pi\hbar}$ corresponding to a intrinsic quantum valley Hall effect. As mentioned\cite{14}, in this regime silicene is a band insulator. These results indicate an electrically tunable phase transition from a topological insulator to a spin valley polarized metal and then to a band insulator, as the electric field increases. It is evident that our results are in agreement with the similar results obtained for the DC spin- and valley-Hall conductivity of silicene in the previous works\cite{21, 22, 23}.

In the doped case, when the Fermi level locate inside the gap, obtained results for $\sigma_{xy}^s$ and $\sigma_{xy}^v$ are similar to those of the undoped case. Then, if an external vertical voltage is applied and increases, a phase transition from a topological insulator to a metal and then to a band insulator occurs\cite{21}. The boundary conditions which limit different phases are represented by $-\Delta_z - \Delta_{so} < \mu < \Delta_z + \Delta_{so}$ and $\Delta_z - \Delta_{so} < \mu < -\Delta_z + \Delta_{so}$ lines for topological insulating phase and $-\Delta_z + \Delta_{so} < \mu < \Delta_z - \Delta_{so}$ or $\Delta_z + \Delta_{so} < \mu < -\Delta_z - \Delta_{so}$ lines for band insulating phase. If the chemical potential increases further such that the Fermi level crosses the lower conduction (upper valance) band, the results become

$$\sigma_{xy}^s = -\frac{e}{4\pi} \left[\frac{\Delta_{so} + \mu}{|\mu|} + 1\right], \quad \sigma_{xy}^v = -\frac{e}{4\pi\hbar} \left[\frac{\Delta_{so} + \mu}{|\mu|} - 1\right]$$

Notice that in this case, unlike the udoped case, silicene shows a nonzero DC response for both
spin- and valley-Hall conductivity which are controlled by $\Delta_{so}$ and $\Delta_z$. While when the Fermi level crosses both conduction (valance) bands, DC spin- and valley Hall conductivity become

$$
\sigma_{xy}^s = -\frac{e}{4\pi|\mu|} \Delta_{so}, \quad \sigma_{xy}^v = \frac{e}{4\pi\hbar|\mu|} \Delta_z. \quad (11)
$$

One can see that in this case the DC spin-Hall conductivity is an intrinsic property and is only controlled by $\Delta_{so}$, whereas the valley-Hall conductivity is arising from and tuned by the applied vertical voltage. Moreover, the direction of the valley Hall conductivity changes by inverting the direction of the applied electric field while the direction of the spin Hall conductivity remains unchanged. These results for the doped case are in agreement with the results reported in the previous works\[21, 22, 23\]. All these results have been summarized in Figs.\[2\] and \[3\] where we have shown the spin and valley Hall conductivity of a electron/hole doped silicene as a function of the vertical electric field and the Fermi energy.

It is evident that in these cases, due to the symmetry of the band structure with respect to interchanging the valley and spin index, there is no spin or valley polarization.

Furthermore, the DC spin- and valley-Hall conductivity of a undoped ferromagnetic silicene can be obtained by making use of Eqs. \[6\] and \[7\]. When the exchange field is less than the minimum gap, at low external vertical voltage, silicene shows a quantum spin Hall effect with an intrinsic quantized Hall conductivity, $\sigma_{xy}^s = -\frac{e}{2\pi}$. By increasing the external vertical voltage silicene becomes metal with nonzero charge- spin- and valley-Hall conductivity. Then at high external vertical voltages a phase transition to a conventional band insulator (characterized by zero charge and spin-Hall conductivities and a nonzero quantized valley-Hall conductivity, $\sigma_{xy}^v = -\frac{e}{2\pi\hbar}$) occurs. The necessary conditions to realize a quantum spin Hall effect are represented by

$$
-\Delta_z - \Delta_{so} < \mu < \Delta_z + \Delta_{so} \quad \text{and} \quad \Delta_z - \Delta_{so} < \mu < -\Delta_z + \Delta_{so}
$$

lines. While the similar conditions for
a quantum valley Hall effect are $-\Delta_z + \Delta_{so} < M < \Delta_z - \Delta_{so}$ or $\Delta_z + \Delta_{so} < M < -\Delta_z - \Delta_{so}$.

Furthermore, when the Fermi level crosses the lower conduction (upper valance) band, our results for the DC spin and valley Hall conductivity become

$$\sigma^{s}_{xy} = -\frac{e}{4\pi} \left[ \Delta_{+,+} \frac{1}{|M|} + 1 \right], \quad \sigma^{v}_{xy} = -\frac{e}{4\pi \hbar} \left[ \Delta_{+,+} \frac{1}{|M|} - 1 \right] \quad (12)$$

Then if the exchange field increases further such that the Fermi level crosses both conduction (valance) bands, DC spin- and valley Hall conductivity become

$$\sigma^{s}_{xy} = -\frac{e}{4\pi} \Delta_{so} \frac{1}{|M|}, \quad \sigma^{v}_{xy} = \frac{e}{4\pi \hbar} \Delta_{z} \frac{1}{|M|}. \quad (13)$$

Note, if the Fermi level crosses both conduction (valance) bands, the DC spin and valley Hall conductivity in a ferromagnetic silicene are intrinsic properties which are controlled only by $\Delta_{so}$ and $\Delta_z$ respectively. Moreover, one can see that in a undoped ferromagnetic silicene similar to the previous case, due to the symmetry of the band structure with respect to interchanging the valley and spin index, any spin/valley polarized transport can not be attained. To achieve a valley or spin polarized transport, one can populate spin or valley states differentially in one valley or spin state. This can be attained, as explained in the following, in a doped ferromagnetic silicene.

Our results for the spin- and valley Hall conductivity in a doped ferromagnetic silicene have been summarized in Fig. 4 and Fig. 5. One can see that the region, in which a quantized spin or valley Hall effect occur, becomes limited when the induced exchange field increases. The necessary conditions to realize a quantum spin Hall effect are represented by $-\Delta_z - \Delta_{so} < \mu < \Delta_z + \Delta_{so}$ and $\Delta_z - \Delta_{so} < \mu < -\Delta_z + \Delta_{so}$ lines. While the similar conditions for a quantum valley Hall effect are $-\Delta_z + \Delta_{so} < M < \Delta_z - \Delta_{so}$ or $\Delta_z + \Delta_{so} < M < -\Delta_z - \Delta_{so}$. 

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Moreover, as mentioned above, a partial or fully spin/valley polarized transport can be captured in a doped ferromagnetic silicene. This can be seen in Fig. 6 and Fig. 7. In Fig. 6 we have shown our results for \( \sigma_{xy}^\uparrow = \sigma_{xy}^K + \sigma_{xy}^{K'} \) and \( \sigma_{xy}^\downarrow = \sigma_{xy}^\downarrow + \sigma_{xy}^{K'} \). The regions, in which \( \sigma_{xy}^\uparrow (\frac{e}{4\pi}) \) or \( \sigma_{xy}^\downarrow (\frac{e}{4\pi}) \) is zero, determine the necessary conditions to realize a fully spin polarized transport. These regions have been shown in Fig. 8. Furthermore, in Fig. 7 the plots of \( \sigma_{xy}^K = \sigma_{xy}^\uparrow + \sigma_{xy}^\downarrow \) and \( \sigma_{xy}^{K'} = \sigma_{xy}^{K'} + \sigma_{xy}^{K'} \), as a function of the vertical electric filed and the chemical potential, have been shown. The regions, in which a fully valley polarized transport can be detected, have been shown in Fig. 8.

4 Summary and conclusions

In summary we studied the intrinsic DC valley and spin Hall conductivity in a ferromagnetic silicene, exploring a fully spin or valley polarized transport. First we calculated its eigenvalues and eigenfunctions. Then, by making use of the Kubo formula, we derived a general relation for the spin and valley Hall conductivity of the ferromagnetic silicene in the presence of finite doping and an electric filed applied perpendicular to its plane. We examined our result by reproducing the results of the previous works in the zero limit of the exchange field. Moreover, we calculated the DC spin and valley conductivity of a doped ferromagnetic silicene. Finally we used our general result to determine the necessary conditions for realizing a fully spin or valley polarized transport.
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Figure 1: The energy spectrum of (a) silicene, and ferromagnetic silicene with $M = \Delta_{so}/2$ when (b) $\Delta_z = 0$, (c) $\Delta_z = \Delta_{so}$ and (d) $\Delta_z = 2\Delta_{so}$.
Figure 2: The transverse spin Hall conductivity, $\sigma_{xy}^{s}(\frac{\mu}{4\pi})$, in a doped silicene as a function of the vertical electric field and the chemical potential.
Figure 3: The transverse valley Hall conductivity, $\sigma_{xy}^{v}(\frac{e}{4\pi\hbar})$, in a doped silicene as a function of the vertical electric field and the chemical potential.
Figure 4: The transverse spin Hall conductivity, $\sigma_{xy}^{s}(\frac{e}{\Delta_{so}})$, in a doped ferromagnetic silicene with $M = \Delta_{so}/2$, as a function of the vertical electric field and the chemical potential.
Figure 5: The transverse valley Hall conductivity, $\sigma_{xy}^v(\frac{e}{4\pi h})$, in a doped ferromagnetic silicene with $M = \Delta_{so}/2$, as a function of the vertical electric field and the chemical potential.
Figure 6: Plots of $\sigma_{xy}^\uparrow\left(\frac{e}{4\pi}\right)$ (top) and $\sigma_{xy}^\downarrow\left(\frac{e}{4\pi}\right)$ (bottom), in a doped ferromagnetic silicene with $M = \Delta_{so}/2$, as a function of the vertical electric field and the chemical potential. The regions in which $\sigma_{xy}^\uparrow\left(\frac{e}{4\pi}\right)$ or $\sigma_{xy}^\downarrow\left(\frac{e}{4\pi}\right)$ is zero determine the necessary conditions to realize a fully spin polarized transport.
Figure 7: Plots of $\sigma^K_{xy}(e^{\frac{e}{4\pi\hbar}})$ (top) and $\sigma^{K'}_{xy}(e^{\frac{e}{4\pi\hbar}})$ (bottom), in a doped ferromagnetic silicene with $M = \Delta_{so}/2$, as a function of the vertical electric filed and the chemical potential. The regions in which $\sigma^K_{xy}(e^{\frac{e}{4\pi\hbar}})$ or $\sigma^{K'}_{xy}(e^{\frac{e}{4\pi\hbar}})$ is zero determine the necessary conditions to realize a fully valley polarized transport.
Figure 8: Regions which determines the necessary conditions to realize a fully spin polarized (FSP) or a fully valley polarized (FVP) transport and also quantum spin Hall effect (QSHE) and quantum valley Hall effect (QVHE). Arrows show how the regions increase or decrease by increasing the exchange field.