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

Yawar Mohammadi [a, *], Borhan Arghavani Nia [b]

[a] Young Researchers and Elite Club, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran
[b] Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

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ABSTRACT

We study intrinsic DC spin and valley Hall conductivity in doped ferromagnetic silicene in the presence of an electric filed 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 transport in ferromagnetic silicene and obtain the necessary conditions for observing a fully spin or valley polarized transport.

1. Introduction

Since successful isolation of a single layer of graphite [1], graphene, as the first real two-dimensional lattice structure which shows novel appealing properties [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 [4], transition metal dichalcogenides (TMDs) [5] and recently a monolayer of silicon, known as silicene [6–9].

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 meV [10,11]. Furthermore, due to the large ionic radius, silicene is buckled [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 nm [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 [11,13–20].

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 [21–25]. 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 [26–28] and MoS_2 [29,31–33], 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 [29]. Moreover as shown by Ezawa

* Corresponding author.
E-mail address: yawar.mohammadi@gmail.com (Y. Mohammadi).

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[30], one can use an off-resonance coherent laser beam to transform silicene from a quantum spin Hall effect or a band insulating into new quantum phases such as photo-induced spin-polarized quantum, spin polarized metal and spin valley-polarized metal, allowing to attain a spin or valley polarized current in silicene. Another way is to apply a vertical external magnetic filed 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 [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 [34–37]. In other way, as in graphene [38,39], the spin/valley polarized current is obtained in silicene [40] 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. Section 2 is devoted to introduce the Hamiltonian model and obtain the general relation for the transverse Hall conductivity. In Section 3 we present our results and discussion. Finally in Section 4 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 [10,40].

$$H_{\eta,s_z} = \hbar v_F\left(k_x\tau_x - \eta k_y\tau_y\right) - \eta s_z\Delta_{so}\tau_z + \Delta_z\tau_z - s_zM, \tag{1}$$

which acts in the sublattice pseudospin space with a wavefunction as $\Psi^{\eta,s_z} = \{\psi_A^{\eta,s_z}, \psi_B^{\eta,s_z}\}^T$. The first part of the Hamiltonian is the Dirac hamiltonian describing the low-energy excitations around Dirac points (**K** and **K**$'$ denoted by η 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 $\Delta_{so} = 3.9$ meV [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 $\Delta_z = E_zd$ where E_z is the electric field and the $2d = 0.46$ nm 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 [41] or from a magnetic insulator substrate like EuO as proposed for graphene [38].

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

$$\varepsilon_\nu^{\eta,s_z} = \nu\sqrt{\Delta_{\eta,s_z}^2 + (\hbar v_Fk)^2} - s_zM, \tag{2}$$

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

$$\Psi_\nu^{\eta,s_z}(\mathbf{k}) = \frac{e^{i\mathbf{k}.\mathbf{r}}}{\sqrt{2\chi_{\eta,s_z}}}\begin{pmatrix}\sqrt{\chi_{\eta,s_z} - \nu\Delta_{\eta,s_z}}\\ \nu\sqrt{\chi_{\eta,s_z} + \nu\Delta_{\eta,s_z}}e^{-i\eta\phi_k}\end{pmatrix}, \tag{3}$$

where $\chi_{\eta,s_z} = \sqrt{\Delta_{\eta,s_z}^2 + (\hbar v_Fk)^2}$ and $\phi_k = \tan^{-1}(k_y/k_x)$. Fig. 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 shows 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, σ_{xy}, written in the Kubo formalism, is given by [42,43].

$$\begin{aligned}\sigma_{xy}^{\eta,s_z} = -i\frac{e^2\hbar}{A}\sum_{\mathbf{k}}\frac{f\left(\varepsilon_+^{\eta,s_z}\right) - f\left(\varepsilon_-^{\eta,s_z}\right)}{\left(\varepsilon_+^{\eta,s_z} - \varepsilon_-^{\eta,s_z}\right)^2}\\ \times\langle\Psi_-^{\eta,s_z}|v_y|\Psi_+^{\eta,s_z}\rangle\langle\Psi_+^{\eta,s_z}|v_x|\Psi_-^{\eta,s_z}\rangle,\end{aligned} \tag{4}$$

where A is the area of the sample and velocity components can be obtained from the Hamiltonian and using relation $v_{k_i} = \frac{1}{\hbar}\frac{\partial H}{\partial k_i}$. Furthermore $f(\varepsilon_\nu^{\eta,s_z}) = 1/(1 + e^{\beta(\varepsilon_\nu^{\eta,s_z} - \mu)})$ is Fermi-Dirac distribution function with μ being the chemical potential