Controllable photo-induced spin and valley filtering in silicene

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Abstract – We study ballistic transport of Dirac electrons through a strip in silicene, when the strip is exposed to off-resonant circularly polarized light and an electric field applied perpendicular to the silicene plane. We show that the conductance through the strip is spin- or/and valley-polarized. This can be explained by spin-valley coupling in silicene, and modification of its band structure through virtual absorption/emission processes and also by the perpendicular electric field. The spin- (valley-) polarization can be enhanced by tuning the light intensity and the value of the perpendicular electric field, leading to perfect spin (valley) filtering for certain of their values. Further, the spin (valley) polarization can be inverted by reversing the perpendicular electric field (by reversing the perpendicular electric field or reversing the circular polarization of the light irradiation). The conditions necessary for the fully valley polarization is determined.

Introduction. – Silicene, a monolayer of silicon atoms arranged in a honeycomb lattice structure, has been synthesized recently \cite{1-4}. Due to large ionic radius of silicon atoms, the honeycomb lattice structure is puckered such that the A and B sublattices are shifted vertically with respect to each other and sit in two parallel planes with a separation of 0.46 nm \cite{5-6}. Due to the puckered structure, which results in a large spin-orbit interaction \cite{7}, the low energy dynamic near the Dirac points in the hexagonal Brillouin zone of silicene is dominated by a massive Dirac Hamiltonian \cite{7}, with a mass which could also be tuned via an electric field applied perpendicular to the silicene plane \cite{5-8}. These novel features donate many attractive properties to silicene \cite{5-8,15}. In silicene, valley and spin degrees of freedom have been coupled via a spin-orbit interaction \cite{7} which is large compared with that in graphene \cite{16}. This can lead to detectable spin- or/and valley-polarized transport in silicene, if the spin or/and valley degeneracies of its band structure are lifted \cite{11-17}. Further, silicon has a long spin-coherence length \cite{18} and spin-diffusion time \cite{19-20}. Motivated by these facts, recently several groups have investigated ballistic transport of Dirac fermions in ferromagnetic silicene junctions \cite{21,22}. They studied the influence of electric and exchange fields on the ballistic transport across single \cite{21,22}, double \cite{22} and arrays \cite{23} of ferromagnetic (FM) barriers. They reported novel results such as perfect spin and/or valley polarization and tunable transport gap which are electrically controllable.

In this letter, we propose a scheme to employ off-resonant circularly polarized light to achieve electrically/optically controllable nearly perfect spin- and valley-filtering in silicene. Our motivation to propose this scheme is the development of new experimental probes \cite{21,24} which make it possible to access non-equilibrium effects arising from off-resonant light irradiation. In our proposed scheme, a strip in a silicene plane is exposed to off-resonant circularly polarized light. Hence, the band structure inside the strip is modified through virtual photon absorption/emission processes, leading to a new energy band which, due to the spin-valley coupling in silicene, is spin-polarized. If a perpendicular electric field is applied, the band structure becomes valley-polarized too. Such a light-irradiated strip can act as a spin- and/or valley-dependent barrier, leading to nearly perfect spin or/and valley filtering for certain values of the light intensity and the perpendicular electric field.

Model Hamiltonian. – We study ballistic transport of Dirac fermions across a strip in a silicene plane, when the strip is exposed to off-resonant circularly polarized light and a perpendicular electric field. Let us take x-axis perpendicular to the edges of the strip (the interfaces) and y-axis along them (see fig. 1). The interfaces are located...
Fig. 1: Schematic of a silicene plane in which a strip (the orange region), is exposed to a perpendicular electric field and off-resonant circularly polarized light.

at $x = 0$ and $x = L$. We also assume the translational invariance along $y$-axis satisfied in the limit of large $W$ (the width of the silicene plane). We restrict our consideration to $W/L \gg 1$ limit, in which the effects of the microscopic details of the upper and lower edges of the silicene plane on the electron transport become insignificant [20].

The low energy excitations in silicene, which occur in vicinity of the Dirac points ($K$ and $K'$), are dominated [27] by a $2 \times 2$ Hamiltonian matrix as

$$H^{\eta,s} = \hbar v_F (k_x \tau_x - \eta k_y \tau_y) - \eta \Delta_{so} \tau_z, \quad (1)$$

acting in the sublattice pseudospin space. The first part of the Hamiltonian is the Dirac Hamiltonian arising from the nearest neighbor transfer energy with $\eta = +$ ($\eta = -$) for $K$ ($K'$). In this term $v_F = \frac{\sqrt{2m_e}}{\hbar}$ is the Fermi velocity with $t = 1.6$ eV and $a = 0.386$ nm being the nearest-neighbor transfer energy and the lattice constant of silicene respectively. $\tau_i$ ($i = x, y, z$) are the Pauli matrices and $k = (k_x, k_y)$ is the two dimensional momentum measured from the Dirac points. The second term is the Kane-Mele term [27] for the intrinsic spin-orbit coupling, in which $\Delta_{so} = 3.9$ meV [7] is the spin-orbit coupling and $s_z$ index referred to two spin degrees of freedom with $s_z = +1$ and $s_z = -1$ for up and down spin degrees of freedom respectively.

As mentioned above, the strip is exposed to a perpendicular electric filed and off-resonant circularly polarized light. Due to the buckled structure of silicene, applying the perpendicular electric field, $E_z$, causes a staggered sublattice potential as $\Delta_z \tau_z$ where $\Delta_z = \epsilon E_z$. The circularly polarized light is described by an electromagnetic potential as

$$A(t) = (\pm A \sin \Omega t, A \cos \Omega t), \quad (2)$$

where $\Omega$ is the frequency of the light and plus (minus) sign corresponds to the right (left) circulation. The gauge potential is periodic in time, $A(t + T) = A(t)$, with the time periodicity $T = 2\pi/\Omega$. The light intensity can be characterized by a dimensionless parameter as $A = e a_A / \hbar$,

$$\Delta H^{\eta,s} = -\frac{[H^{\eta,s}, H^{\eta,s}]}{\hbar \Omega} + \mathcal{O}(A^4), \quad (3)$$

where $H^{\eta,s} = (1/T) \int_0^T e^{-i\Omega t} H^{\eta,s}(t) dt$. It is easy to show that $[H^{\eta,s}_1, H^{\eta,s}_2] = \pm (h v_F)^2 A^2 \tau_z / a^2$ with $+(-)$ for right (left) circulation. Hence the low energy dynamics in silicene, in the presence of off-resonant circularly polarized light irradiation and an electric filed applied perpendicular to the silicene plane, are dominated by an effective Hamiltonian as

$$H_{\text{eff}}^{\eta,s} = H^{\eta,s} + \Delta_z \tau_z - \eta \Delta_{\Omega} \tau_z, \quad (4)$$

acting in the sublattice pseudospin space where $\Delta_{\Omega} = \pm (h v_F)^2 A^2 / a^2 \hbar \Omega$ with $+(-)$ for right (left) circulation. The corresponding energy bands are obtained by diagonalizing the Hamiltonian, Eq. (4) which are given by

$$\varepsilon_{\eta,s} = \nu \sqrt{(h v_F |k|)^2 + \Delta^2}, \quad (5)$$

where $\Delta = \Delta_z - \eta \Delta_{so} = \eta \Delta_{\Omega}$ and $\nu = +(-)$ denotes to the conduction (valance) band. The low energy bands, in the regions I and III, are obtained from Eq. (4) by just setting $\Delta_z = 0$ and $\Delta_{\Omega} = 0$.

The wave functions in the different regions (see fig. 1) can be written in terms of the incident and reflected waves. In the regions I and III, they are

$$\psi_{\nu}^{\eta,s} = e^{ik_{so} x} e^{i k_{so} y} \frac{1}{2\chi} \left( \begin{array}{c} \sqrt{\chi - \nu \Delta_{so}} \\ \nu e^{-i \phi} \sqrt{\chi + \nu \Delta_{so}} \end{array} \right), \quad (6)$$

in the region I and

$$\psi_{\nu}^{\eta,s} = t_{\eta,s} e^{i (k_{so} x + k_{so} y) / 2\chi} \left( \begin{array}{c} \sqrt{\chi - \nu \Delta_{so}} \\ \nu e^{-i \phi} \sqrt{\chi + \nu \Delta_{so}} \end{array} \right), \quad (7)$$

in the region III, where $\nu = +(-)$ denotes to the conduction (valance) band, $\chi = \sqrt{(h v_F |k|^2 + \Delta_{so}^2}$, $\theta = \tan^{-1} (k_y / k_x)$ is the angle of incidence and $r_{\eta,s}$, and $t_{\eta,s}$ are the reflection and the transmission coefficients respectively. The corresponding wave function, in the strip (region II), is given by

$$\psi_{\nu}^{\eta,s} = e^{i q_y a_{\eta,s}} e^{i q_x z} \left( \begin{array}{c} \sqrt{\chi - \nu \Delta} \\ \nu e^{-i \phi} \sqrt{\chi + \nu \Delta} \end{array} \right).$$
where \( \chi' = \sqrt{(\hbar v_F |q|)^2 + \Delta^2} \) and \( \phi = \tan^{-1}(q_y/q_x) \) is refractive angle inside the strip with \( q = (q_x, q_y) \) being the two dimensional momentum. The coefficients \( a_{\eta,s} \) and \( b_{\eta,s} \) could be determined by requiring continuity of the wave functions and their derivatives at the interfaces.

We restrict our calculations to the elastic scattering at the interfaces. Hence, the translational invariance along \( y \)-axis implies conservation of the transverse momentums outside the strip, \( k_y \), and inside it, \( q_y \), which yields \( k_F \sin \theta = q_F \sin \phi \), where

\[
  k_F = (k_x^2 + k_y^2)^{1/2} = (\hbar v_F)^{-1} \sqrt{\varepsilon_F^2 - \Delta_{so}^2},
\]

and

\[
  q_F = (q_x^2 + q_y^2)^{1/2} = (\hbar v_F)^{-1} \sqrt{\varepsilon_F^2 - \Delta^2},
\]

with \( k_F \) and \( q_F \) being the Fermi momentum outside and inside the strip respectively with \( \varepsilon_F \) being the Fermi energy. The coefficients of the incident and reflected wave functions could be determined by requiring continuity of the wave functions and their derivatives at the interfaces. Matching the wave functions and their derivatives yield same results. So, we only need to match the wave functions at the interfaces, \( x = 0 \) and \( x = L \), which ensures the conversion of the local current at the interfaces too. These conditions yield

\[
  t_{\eta,s} = (\cos(q_x L) - i\mathcal{F}(k_F, \theta) \sin(q_x L))^{-1},
\]

for the transmission coefficient through the strip where

\[
  q_x = k_F \sqrt{\frac{\varepsilon_F^2 - \Delta^2}{\varepsilon_F^2 - \Delta_{so}^2} - \sin^2 \theta},
\]

and

\[
  \mathcal{F}(k_F, \theta) = \frac{k_x^2 - \varepsilon_b^2 + q_x^2 - \varepsilon_b^2 + k_y^2 - \varepsilon_b^2}{2\varepsilon_b k_x q_x},
\]

with \( k_x = k_F \cos \theta, \varepsilon_l = \varepsilon_F + \Delta_{so} \) and \( \varepsilon_b = \varepsilon_F + \Delta \). Here we remark a point worth mentioning. Note that for \( q_x L = n\pi \), with \( n \) being an integer number, the transmission is perfect, called Fabry-Pérot resonance. This occurs when \( n \) times half the wavelength of the wave inside the barrier is equal to the length of the strip.

Spin- and valley-resolved conductance in the Landau-Büttiker formalism are given by

\[
  G_{\eta,s} = \frac{G_0}{2} \int_{-\pi/2}^{\pi/2} T_{\eta,s}(k_F, \theta) \cos \theta d\theta,
\]

where \( G_0 = \frac{4e^2 W}{h} \) and \( W \) is the width of the silicene sheet. To explore the spin/valley polarization through the strip, we define the spin and valley polarization as \( P_x = (G_\uparrow - G_\downarrow)/(G_\uparrow + G_\downarrow) \) and \( P_y = (G_K - G_K')/(G_K + G_K') \) respectively where \( G_{\eta,s} = \sum_q G_{q,\eta,s} \) and \( G_\eta = \sum_q G_{q,\eta,s} \).

So, \( P_x = +1(-1) \) corresponds to a current which is carried entirely by spin-up (spin-down) electrons, while \( P_y = +1(-1) \) corresponds to a current that is carrier by the electrons localized completely in the \( K(K') \) valley. The total charge conductance is obtained by summing \( G_{\eta,s} \) over \( s \) and \( \eta \).

**Results and Discussion.** – In this section we present our results for conductance, spin and valley polarizations and use them to discuss off-resonant photo-induced spin- and valley-filtering in silicene. We first discuss it in the absence of the perpendicular electric field (\( \Delta_z = 0 \)) and then in its presence (\( \Delta_z \neq 0 \)).

\( \Delta_z = 0 \): In the presence of off-resonant light irradiation, the energy bands are modified through virtual photon absorption/emission processes. Such photon-dressed bands in silicene, due to the spin-valley coupling, become spin-polarized. So if the light intensity is tuned properly, the conductance trough the strip can becomes partially or even fully spin-polarized provided the Fermi level crosses the conduction (or valance) bands. We have plotted in fig. 2 the spin-resolved conductance through the strip, \( G_\uparrow \) (solid black curves) and \( G_\downarrow \) (dashed blue curves), as a function of \( L \) for two different values of \( \Delta, \Delta = 8.0\Delta_{so} \) (right panel) and \( \Delta = 12.0\Delta_{so} \) (left panel). The Fermi energy for both left and right panels is \( \varepsilon_F = 12.0\Delta_{so} \).

In the left panel, both \( G_\uparrow \) and \( G_\downarrow \) exhibit an oscillatory decaying dependence on the length of the strip, without being completely suppressed even for large \( L \). This can be explained by the band structure of the silicene inside the strip, in which the Fermi level crosses both spin-up and spin-down electron bands (see fig. 2(b)), leading to propagating modes inside the strip for both spin wave functions. Further, left panel of fig. 2 shows a partially spin polarization which can be enhanced by increasing \( \Delta \), leading to a fully spin polarization as seen in the right panel in which \( G_\downarrow \) decays with \( L \) in an oscillatory way while \( G_\uparrow \) is strongly suppressed if the length of the strip is large enough. This is due to the fact that the Fermi level crosses only the spin-down energy band around each Dirac point inside the strip (see fig. 3(c)), satisfied when \( \Delta \) becomes larger than a critical value, \( |\Delta_{\uparrow}| = \varepsilon_F - \Delta_{so} \). Hence, \( q_x \) becomes imaginary leading to monotonically decaying the transmission probability and consequently the spin-resolved conductance in terms of \( L \) (see Eqs. 11,12).

The spin polarization could be inverted by reversing the polarization of the light. Because changing circular polarization of the light from right to left polarization or vice versa interchanges the spin-up and spin-down electron bands in the strip. This is clear from the fig. 3 in which we have plotted the spin polarization as a function of \( \Delta \) for different values of the Fermi energies, \( \varepsilon_F = 8\Delta_{so}, \varepsilon_F = 12\Delta_{so} \) and \( \varepsilon_F = 16\Delta_{so} \). This figure, with the band structure of silicene inside the strip, can also be used to determine the necessary condition to realize a fully spin.
polarization. This condition is $\varepsilon_F - \Delta_{so} < |\Delta_\Omega| < \varepsilon_F + \Delta_{so}$ and $\varepsilon_F > \Delta_{so}$. The results presented in figs. 4 and 5 reveal off-resonant photo-induced perfect spin filtering in silicene.

$\Delta_z \neq 0$: Applying a perpendicular electric ($\Delta_z \neq 0$) lifts the valley-degeneracy of the energy bands (see Eq. 5). So, in addition to a spin polarization, one can achieve a partially valley polarization. The partially spin/valley polarization can be enhanced, giving rise to a fully spin/valley polarization. This can be done by changing the intensity of the light (and consequently $\Delta_\Omega$) for a non-zero value of the constant $\Delta_z$ or vise versa. Figure 5 displays the spin-resolved (left panel) and the valley-resolved (right panel) conductances across the strip as functions of $\Delta_\Omega/\Delta_{so}$ for $\Delta_z = 4\Delta_\Omega$ when $\varepsilon_F = 12\Delta_\Omega$ and $L = 100 \text{ nm}$. Let us first consider the dependence of the spin polarization on $\Delta_\Omega$ and $\Delta_z$, and appearance of a fully spin polarization in the left panel. This can be understood by the band structure in the strip. With changing $\Delta_\Omega$, the energy bands and consequently the hight of the barrier in the strip are changed, leading to change in the transmission probability and consequently the charge conductance. If $\Delta_\Omega$ increases such that the bottom of an energy band approaches (leaves) the Fermi level, its carrier concentration decreases (increases). Hence, the conductance arising from that energy band decreases (increases). Once the Fermi level crosses the bottom of an energy band and locates inside its energy gap, the conductance, arising from that energy band, is suppressed completely. So, the total conductance (the spin- or valley-resolved conductance in fig. 5) decreases intensively. Such a decrease takes place at $\Delta_\Omega = 7\Delta_{so}$ ($\Delta_\Omega = 9\Delta_{so}$) for $G^\uparrow$ ($G^\downarrow$) in left panel of fig. 5 where the Fermi level crosses the bottom of $\varepsilon_{K^\uparrow}$ ($\varepsilon_{K^\downarrow}$) band and locates in its energy gap. This happens when $\varepsilon_F = [|\Delta| = |\Delta_z + \eta(s_3\Delta_{so} + \Delta_\Omega)|]$. If $\Delta_\Omega$ increases further and becomes larger than a critical value ($\Delta_\Omega = 15\Delta_{so}$), the Fermi level locates inside the gap of $\varepsilon_{K^{'\uparrow}}$ band too satisfied when $\varepsilon_F < |\Delta_z + (-)(+\Delta_{so} + \Delta_\Omega)|$. In this situation the Fermi level only crosses $\varepsilon_{K^{'\downarrow}}$, so the current is entirely carried by the spin down electrons near the $K'$ point.

Similarly, the dependence of $G_K$ and $G_{K'}$ on $\Delta_\Omega/\Delta_{so}$ (in the right panel of fig. 5) can be explained. If $\Delta_\Omega$ becomes larger than $8\Delta_{so}$, happened when the Fermi level locates inside the gap of both $\varepsilon_{K^\uparrow}$ and $\varepsilon_{K^{'\downarrow}}$ energy bands, the current is entirely carried by the electrons near $K$ point. So, the current becomes fully valley polarized.

In the presence of the perpendicular electric field, the spin and the valley polarization can be inverted by changing the direction of the applied electric field (determined by the sign of $\Delta_z$) and also by changing the polarization of the light (determined by the sign of $\Delta_\Omega$). This is clear from figs. 6 and 7 in which we have plotted spin-resolved (left panel) and valley-resolved (right panel) conductances as functions of $\Delta_z/\Delta_{so}$.

Summary and conclusions. – In summary, we studied ballistic transport of Dirac electrons through a strip in silicene, when the strip is exposed to off-resonant circularly polarized light and an electric field applied per...
perpendicular to the silicene plane. We showed that the spin- and valley-conductance through the strip is polarized. This can be understood by the spin-valley coupling in silicene via a strong spin-orbit interaction, and modification of its band structure by photon dressing process and the perpendicular electric field. The spin (valley) polarization of the current can be enhanced by tuning the light intensity and the value of the perpendicular electric field. The spin (valley) polarization can be inverted by reversing the perpendicular electric field (by reversing the perpendicular electric field or reversing the circular polarization of the light irradiation).

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Fig. 6: (a) Spin-resolved conductance and (b) Valley-resolved conductance as a function of $\Delta z/\Delta so$. The other parameters are $\varepsilon_F = 12\Delta so$, $\Delta\Omega = 6\Delta so$ and $L = 100 \text{ nm}$.

Fig. 7: Counter plot of spin polarization, $P_s$, as functions of $\Delta\Omega/\Delta so$ and $\Delta z/\Delta so$. The other parameters are $\varepsilon_F = 12\Delta so$ and $L = 100 \text{ nm}$.

Fig. 8: Counter plot of valley polarization, $P_v$, as functions of $\Delta\Omega/\Delta so$ and $\Delta z/\Delta so$. The other parameters are $\varepsilon_F = 12\Delta so$ and $L = 100 \text{ nm}$.