Generation of a fully valley-polarized current in bulk graphene

Yu Song,† Feng Zhai,‡ and Yong Guo

1 Institute of Electronic Engineering, China Academy of Engineering Physics, Mianyang 621900, P. R. China
2 Center for Statistical and Theoretical Condensed Matter Physics and Department of Physics, Zhejiang Normal University, Jinhua 321004, P. R. China
3 Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, P. R. China

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The generation of a fully valley-polarized current (FVPC) in bulk graphene is a fundamental goal in valleytronics. To this end, we investigate valley-dependent transport through a strained graphene modulated by a finite magnetic superlattice. It is found that this device allows a coexistence of insulating transmission gap of one valley and metallic resonant band of the other. Accordingly, a substantial bulk FVPC appears in a wide range of edge orientation and temperature, which can be effectively tuned by structural parameters. A valley-resolved Hall configuration is designed to measure the valley polarization degree of the filtered current.

In this Letter we present a scheme to achieve a fully valley-polarized current (FVPC) in bulk graphene. The proposed valley filter is a strained graphene under a periodic magnetic field and a uniaxial tensile strain. The low-energy electronic elementary excitations in bulk graphene originate from the out-of-plane $p_x-p_y$ hybridization. Their massless energy dispersion is well described by Dirac cones at the six corners of the Brilliouin zone. The six cones can be divided into two inequivalent groups labeled by the valley index $K$ and $K'$. Intervaly coupling or scattering requires a rather large change of the momentum and is thus suppressed in clean graphene samples. This independence suggests that the valley degree of freedom could be utilized as an information carrier.

How to generate a high-contrast valley population of charge carriers is a fundamental goal of graphene valleytronics. Several proposed valley filters require either a point contact with zigzag edges or a breaking of the inversion symmetry. These factors may break the specific bulk elementary excitation that is essential for most of the excitement about graphene. Such Klein tunneling, nonzero minimum conductivities, and half-integer quantum Hall effect. Therefore, several schemes of valley filtering have been proposed based on bulk graphene, utilizing either valley-dependent trigonal band warping, or pseudo magnetic fields induced by strain. However, the generated valley polarization is shown to be low even at zero temperature.

In this Letter we present a scheme to achieve a fully valley-polarized current (FVPC) in bulk graphene. The proposed valley filter is a strained graphene under a periodic magnetic modulation. We show that the combination of the periodic magnetic field and the strain can lead to a coexistence of insulating transmission gap of one valley and metallic resonant band of the other. Under this mechanism, the bulk FVPC survives in a wide range of edge orientation, temperature, and structural parameters. We also discuss how to measure the valley polarization degree of the output current.

Suppose that the magnetic superlattice consists of $n$ ferromagnetic metal (FM) strips. Each FM strip $j$ $(1 \leq j \leq n)$ has a size $L_F$ along the $x$ direction, a magnetization $M = Me_z$, a distance $L_S$ to the nearest strip(s) [see Fig. 1(b)], and is close enough to the graphene plane. The induced magnetic field can be approximately described by the vector potential

$$A_M(r) = \sum_j A_M(x - x_j^M)\Theta(x_j^S - x)e_y.$$  

Here $\Theta(x)$ is the Heaviside step function, $x_j^S = x_j^S + L_S + L_F$ the size of a unit cell, and $x_j^M = x_j^S - L_F$. The uniaxial tensile strain is homogeneous in the whole filtering region, i.e., $u_{yy} - u_{xx} = u$ and $u_{xy} = 0$. It leads to changes in the nearest-neighbor hopping amplitudes, and can be described by pseudo magnetic vector potentials. When the edge orientation (the $x$-axis) has an angle $\beta$ with respect to the armchair direction $Ox_0$ [see Fig. 1(c)], the pseudo vector potential reads

![FIG. 1. (a) Schematic diagram of the strained graphene modulated by a finite magnetic superlattice. The bulk graphene sample is placed on a substrate in the $(x,y)$ plane. In the filtering region the substrate is subject to a uniaxial tension along the $x$-direction. The periodic magnetic field is created by a finite superlattice of $n$ ferromagnetic metal (FM) strips depositing on top of the filtering region. (b) The last two unit cells of the superlattice (top view). To measure the degree of the valley polarization, a gapped region is connected to the considered structure from the right. (c) The edge orientation angle $\beta$.](image-url)
Here $G$ is the conductance per valley. In the low-energy continuum approximation, the Hamiltonian for a given valley is

$$H = v_F p \cdot (p + eA_M + \lambda \psi(x, y)),$$

where $\lambda = \pm$ for the valley $K$ and $K'$, $v_F$ is the Fermi velocity, $\sigma = (\sigma_x, \sigma_y)$ is the pseudospin Pauli matrices, and $p$ is the momentum operator. For brevity, here we express all quantities in dimensionless form by means of a characteristic length $l_0 = 10$ nm and energy unit $E_0 = h v_F / l_0 = 56.55$ meV. We assume that the sample width $W >> L'$ so that edge details are not important. For an electron with energy $E$ and incident angle $\alpha$, the envelope function in each region $(i = N, S, M)$ of the building block $j$ has the form

$$\psi_{ij}(r) = e^{i q_y y} \Theta(x) \hat{\Theta}(L' - x) \psi(x, y) dx,$$

where $\Theta(x) = 1$ for $x > 0$ and $0$ for $x < 0$. The wave amplitudes $u_{ij}$ and $v_{ij}$ are determined from the continuity of the envelope function and the scattering boundary condition $u_{N,0} = 1$ and $v_{N,n+1} = 0$. We write

$$M_{ij} = \left( \begin{array}{cc} u_{S,j+1} & u_{S,j} \\ v_{S,j+1} & v_{S,j} \end{array} \right),$$

$$M_1 = \frac{a}{c} \left( \begin{array}{cc} a & b \\ c & d \end{array} \right),$$

where $M_j$ $(1 \leq j \leq n)$ is the transfer matrix for the superlattice unit cell $j$. By means of the matrix $U_i(x) = [\phi_+^1(x), \phi_-^1(x)]$ and the condition $\psi_{S,j+1}(x^*_j) = \psi M_j(x^*_j)$ and $\psi_{M,j}(x^*_M) = \psi S_j(x^*_M)$, one can express $M_j$ as

$$M_j = U^{-1} S_j U M_j S_j U^{-1} M_j S_j U,$$

From Eq. (3) we get det $M_j = 1$ and the matrix element $M_{21}^j = a$, $M_{11}^j = \tau^{-1} - b$ with $\tau = e^{-2i k s L'}, M_{12}^j = 1$ and $M_{22}^j = d$. Here we have used the identity $U_i(x + i) = U_i(x) \delta \{e^{i k s L'}, e^{-i k s L'}\}$. The transfer matrix for the finite superlattice is $N_m = M_{N} \cdots M_2 M_1 = [a_{mn}, c_{mn}] T_{mn}, (b_{mn}, d_{mn}) T_{mn}$. From the recurrence relation $N_{j+1} = M_{j+1} N_j$ and $N_1 = M_1$, we obtain the matrix elements of $N_m$

$$a_n = \frac{1}{2} (F^n + G^n) + \frac{a - \tau d}{2D} (F^n - G^n),$$

$$b_n = \frac{\tau^{-1} c_n}{1 - \frac{\tau}{D} (F^n - G^n)},$$

$$\tau^n d_n = \frac{1}{2} (F^n + G^n) - \frac{a - \tau d}{2D} (F^n - G^n).$$

Here $B = a + \tau d$, $D = \sqrt{B^2 - 4\tau}, F = (B + D)/2$, and $G = (B - D)/2$. The total transfer matrix $M = U^{-1} N_{N} U S(L') N_{N} U S(L') U_{N,0} U_{S,0} U_{N,0}$ determines the valley-resolved transmission coefficient $t_\xi = u_{N,n+1} = 1/M^{22}$. The transmission probabilities read

$$T_\xi(E, q) = |\xi|^2 = \left| \frac{4k_N k_S}{\lambda_s a_n + \lambda_b b_n + \lambda_c c_n + \lambda_d d_n} \right|^2,$$

where $\lambda_s = [- (k_N - k_S)^2 - \Delta^2] e^{2ik_s L'}$, $\lambda_b = [k^2_S - (k_N - i\Delta)^2] e^{2ik_s L}$, $\lambda_c = [- k^2_N + (k_N + i\Delta)^2] e^{2ik_s L}$, $\lambda_d = (k_N + k_S)^2 + \Delta^2$, and $\Delta = q_N - q_S$.

Recent mobility measurements on graphene indicate that the electron-phonon scattering can be ignored in the temperature range of 10K-100K. In this range, the ballistic valley-resolved conductance is given by the Landau-Büttiker formula

$$G_\xi(E_F, T_F) = G_0 \int d E d \frac{d \theta}{d E} \int_{- E_F}^{E_F} T_\xi(E, q) dq \frac{d E}{2\pi},$$

where $f(E) = [1 + (E - E_F)/T_F]^{-1}$ is the Fermi-Dirac distribution function at the temperature $T_F$ and the Fermi energy $E_F$, and $G_0 = 2e^2/h$ is the quantum conductance (2 accounts for the spin degeneracy). The zero-temperature conductance can be rewritten as $G_\xi(E_F, 0) = MG_0 [(E_F - E)/T_F] T_F(E_F, \alpha) \cos \alpha d \alpha$, where $M = (1 + (E_F)/E_0)(W/2\pi a_0) M_F M_W$ is half of the number of the transverse modes and $2MG_0$ is the maximal channel conductance per valley.

In Fig. 2 we present the results for $T_F = 0$ and $\beta = 0$. As the incident energy decreases, the transmission demonstrates obvious quasi transparent region and transmission gap [see Figs. 2(a) and 2(b)]. The transmission gap is divided into two parts by a resonant region of
The generation mechanism is rather small conductance makes it impossible for either the valley polarization is as good as in the window II, the current from valley \( K' \) is almost totally blocked while \( K \) is high [Fig. 2(c)]. Actually, for \( \beta = \pi/6 \) (the zigzag direction), the valley polarization completely disappears because \( G_{-\xi}(\beta) = G_{\xi}(\pi/3 - \beta) \) [Figs. 3(c) and 3(d)]. A remarkable FVPC (high VDO with substantial \( G \)) can be obtained under \( \beta \approx 0 \) and relatively high Fermi energies. It can be also achieved under \( \beta \approx \pi/9 \) and relatively low Fermi energies. Under such \( \beta \) values, electrons in valley \( K' \) feel alternate modulations of total vector potential \( \mp A_x \cos 3\beta \) along the \( x \) direction, which lead to an almost transparent transmission [dashed curves in Fig. 3(d)]. In the following we will focus only on the armchair edge (\( \beta = 0 \)).

We now consider the effect of temperature, which is
shown in Fig. 3. The rich oscillations in the conductance spectrum at zero temperature are gradually smeared out as the temperature increases. Generally, the valley currents decrease (increase) with the temperature in the resonant bands (blocked regions). This leads to increasing total current in window I and decreasing VDO in window II (see Fig. 3(a) (b)). As a result, both windows I and II become smaller and disappear with the increase of temperature (see Fig. 3(c)). These behaviors can be understood from Eq. (3). Valley currents at a finite temperature \( T_P \) are determined by the zero-temperature valley currents in an estimated energy range \( \sim (E_F - 5T_P, E_F + 5T_P) \). In this range a dramatic variation of \( G \) (\( T_P = 0 \)) with energy results in an obvious temperature effect. Nevertheless, we can still obtain a bulk FVPC in a wide range of Fermi energy at a low temperature [see Fig. 3(c)].

The tunability of a FVPC source is desirable for valleytronics applications. In Fig. 4, we examine the influences of structural parameters such as the number \( n \) of superlattice units and the strain strength \( A_S \). For simplicity, the ratio \( A_S : A_M \) and \( L_S : L_F \) are fixed at 1:1. When \( n \) increases from 5 to 10, the total conductance is lowered slightly and more conductance peaks appear [see Eq. (4)]. As the optimal VDO increases greatly, we can obtain bulk FVPC at higher temperatures in an almost unchanged energy window. However, the choice of \( n \) should guarantee that the total length is smaller than the electron mean free path and valley coherent length. With the increasing of \( A_S \), bulk FVPC can appear in a wider Fermi energy window and the optimal VDO also increases, while the conductance decreases greatly. Thus the strain (and magnetization) strength should be chosen as moderate. All the results above are obtained under electron-hole symmetry. If this symmetry is broken by a common negative gate voltage on all FM strips, the conductance in the hole (electron) region increases (decreases) but the VDO decreases (increases). Both the conductance and VDO curves shift towards the hole region. As a result, the inclusion of a negative (positive) electric potential is helpful for obtaining bulk FVPC for electrons (holes) in lower energy and at higher temperature.

The injection of a valley-polarized current into a gapped graphene will lead to a finite Hall voltage. This mechanism can be utilized to measure the valley polarization degree of the filtered current [see Fig. 1(b)]. Due to the effective valley dependent gaps [5] \( G_K' (G_K) \) changes slightly to \( G'_K (G_K) \) in the detection region. The voltage between the upper (lower) edge and the middle region \( V_1 (V_2) \) is proportional to \( G'_K (G_K) \). Thus \( P \) and VDO can be respectively reflected by \( (V_2 - V_1)/(V_2 + V_1) \) and \( \log(V_2/V_1) \), especially when the gap is small. A rather huge positive (negative) \( \log(V_2/V_1) \) is an evidence for that we obtain a FVPC of valley \( K' (K) \).

In summary, we have demonstrated that a strained graphene under the modulation of a finite magnetic superlattice can generate a bulk FVPC. The FVPC appears in a wide range of edge orientation angles and temperature. The underlying mechanism is the coexistence of the metallic resonant band and insulating transmission-blocked region of two valleys in a certain Fermi energy window. Such a mechanism implies that superlattices consisting of any valley filtering structures can be used to generate a FVPC. The FVPC can be effectively controlled by tuning the structural parameters, and may be used as a high-quality current source of bulk valleytronics. A valley-resolved Hall configuration is suggested to measure the valley polarization degree of the filtered current.

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\*kwungvusung@gmail.com
†fzhai@pku.cn

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[20] Note that the change is not due to the edge’s microscopic termination which alter with the edge orientation, because the sample under consideration is sufficiently wide hence bulk states dominate the valley-resolved transport. Due to this factor and large Fermi wavelength at small $E_F$ (see Ref. [3]), edge imperfections can be also ignored.