Doctopic: Condensed matter ARTICLE IN PRESS PLA:24807

Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Valley filtering due to orbital magnetic moment in bilayer graphene

Chang-Soo Park

Department of Physics, Dankook University, Cheonan 330-714, Republic of Korea

ARTICLE INFO

Article history:
Received 27 September 2017
Received in revised form 18 October 2017
Accepted 22 October 2017
Available online xxxx
Communicated by M. Wu

Keywords:
Valley filtering
Orbital magnetic moment
Bilayer graphene

ABSTRACT

We investigate the effect of valley-dependent orbital magnetic moment on the transmission of quasiparticles through biased bilayer graphene *npn* and *pnp* junctions in the presence of out-of-plane magnetic field. It is shown that the valley-polarized Zeeman-like energy splitting, due to the interaction of orbital magnetic moment with magnetic field, can suppress the transmission of quasiparticles of one valley while transmitting those of the other valley. This valley-selective transmission property can be exploited for valley filtering. We demonstrate that the *npn* and *pnp* junction, respectively, filters off the K'-valley and K-valley particles, with nearly perfect degree of filtration.

1. Introduction

Valley pseudospin, an extra intrinsic degree of freedom in 2D materials such as graphene and transition metal dichalcogenides, has drawn much attention in recent years because of its potential application as information storage, known as valleytronics. To utilize the valley degree of freedom it is essential to produce valley-polarized particles by breaking inversion and/or time-reversal symmetries. Various theoretical proposals for valley filtering have been made in monolayer (MLG) and bilayer (BLG) graphenes, which include the effects of quantum point contact [1,2], trigonal warping [3–5], strain due to mechanical deformation [6–12], line defects [13–15], electromagnetic waves [16,17], combination of MLG and BLG [18], or substrate-induced mass [19–21]. One of the primary issues in this subject is to find an effective and controllable way of valley filtering.

In this paper, we propose a different mechanism that can facilitate the valley filtering with high efficiency. Our model is based on Zeeman-like interaction between orbital magnetic moment of quasiparticles in BLG and external magnetic field. As the valley pseudospin represents degenerate states of the two different symmetry points K and K' in momentum space it is intimately related to the Berry phase [22]. In association with the Berry phase there are also two physically observable quantities, Berry curvature and orbital magnetic moment [23,24]. The Berry curvature can exist when a crystal has broken inversion symmetry (and/or broken time-reversal symmetry) [25,26] and the orbital magnetic moment stems from the self rotation of wavepacket in semiclassical description of quasiparticles in a band. A unique feature of these quantities in graphene is that both of them depend on the valley degree of freedom, carrying valley-dependent electronic and transport properties [23,27–32].

In the presence of an external magnetic field the orbital magnetic moment interacts with the field to induce Zeeman-like energy shift in a band. The energy shift has opposite signs at different valleys due to the valley dependence of orbital magnetic moment, called a valley Zeeman effect [23]. Exploiting this valley-contrasting energy shift we investigate its effect on the transmission of quasiparticles through biased BLG *npn* (barrier) and *pnp* (well) junctions with out-of-layer magnetic field applied in the barrier/well regions. When quasiparticles pass through a junction they will experience the energy shift due to the valley Zeeman effect. Because of the opposite polarity of the K and K' valleys, the energy of one valley may enter band gap, while that of the other valley stays within band. Below, we demonstrate that the transmission of quasiparticles with energies inside a band gap can be greatly suppressed, whereas those within a band will pass through the junctions with large probabilities. As a result, the junctions can filter off quasiparticles of one valley while transmitting those of the other valley, exhibiting valley filtration.

2. Valley-dependent Zeeman effect

In this section we discuss about the valley Zeeman effect in bilayer graphene with band gap. Let us consider a bilayer graphene (BLG) biased by external gate voltages. The low-energy effective two-band Hamiltonian of the BLG can be expressed as [33–35]

$$\hat{\mathcal{H}}_0 = -\frac{p_x^2 - p_y^2}{2m^*}\hat{\sigma}_x - \tau\frac{\{p_x, p_y\}}{2m^*}\hat{\sigma}_y + u\hat{\sigma}_z\,, \tag{1}$$

E-mail address: olnal@dankook.ac.kr.

https://doi.org/10.1016/j.physleta.2017.10.044
0375-9601/© 2017 Elsevier B.V. All rights reserved.

where $\{p_x, p_y\}$ denotes anticommutation ($p_{x,y} = -i\hbar\partial_{x,y}$), $\hat{\sigma}_i$ ($i = x, y, z$) are Pauli matrices, $m^* = \gamma_1/2v_F^2$ is an effective mass ($\gamma_1 \approx 0.4$ eV, $v_F \approx 10^6$ m/s), τ is the valley index with $\tau = +1$ for the K valley and $\tau = -1$ for the K' valley, and u is a half of gap ($u = \Delta/2$ with Δ being the gap) due to the bias. Transforming the Hamiltonian, $\hat{\mathcal{H}}_0(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\hat{\mathcal{H}}_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, for an adiabatic process in the $\boldsymbol{k}$-space [23], we can construct an eigenvalue equation

$$\hat{\mathcal{H}}_0(\boldsymbol{k})|\chi_{s\tau}(\boldsymbol{k})\rangle = \epsilon_s(\boldsymbol{k})|\chi_{s\tau}(\boldsymbol{k})\rangle\,, \tag{2}$$

where $\epsilon_s = s\epsilon$ with $s = \pm 1$ bing the band index. The energy and pseudospinor are given by

$$|\chi_{s\tau}\rangle = \frac{1}{\sqrt{2\epsilon}}\begin{pmatrix}\sqrt{\epsilon + su}\\ -se^{2i\tau\phi}\sqrt{\epsilon - su}\end{pmatrix}, \quad \epsilon = \sqrt{\epsilon_k^2 + u^2}\,, \tag{3}$$

where $\phi = \arctan(k_y/k_x)$ and $\epsilon_k = \hbar^2k^2/2m^*$ with $k^2 = k_x^2 + k_y^2$. Owing to the diagonal term $u\hat{\sigma}_z$ in the Hamiltonian (1) space-inversion symmetry is broken in biased BLG. It is thus possible to have non-zero Berry curvature. Using Eq. (3) the Berry curvature, which is a gauge invariant quantity, for the biased BLG can be obtained as follows:

$$\begin{aligned}\boldsymbol{\Omega}_{s\tau} &= i\langle\nabla_k\chi_{s\tau}| \times |\nabla_k\chi_{s\tau}\rangle\\ &= -s\tau\frac{\hbar^2}{m^*}\frac{u\sqrt{\epsilon^2 - u^2}}{\epsilon^3}\,\hat{\mathbf{e}}_z\,.\end{aligned} \tag{4}$$

The dynamics of quasiparticles in a band s can also be described by semiclassical equation of motion of a wavepacket [36]. In this case, due to the finite spread of wavepacket, the self rotation of wavepacket about its center can produce an orbital magnetic moment [23]. For BLG, using the particle–hole symmetry [27,37], the orbital magnetic moment can be obtained from the Berry curvature via following relation:

$$\boldsymbol{\mathcal{M}}_\tau = s\epsilon\frac{e}{\hbar}\boldsymbol{\Omega}_{s\tau} = -\tau\mu_B^* f(\epsilon, u)\hat{\mathbf{e}}_z\,, \tag{5}$$

where μ_B^* is an effective Bohr magneton defined as $\mu_B^* = e\hbar/2m^* \approx 1.7$ (meV/T) and we have introduced an energy function

$$f(\epsilon, u) = \frac{2u}{\epsilon^2}\sqrt{\epsilon^2 - u^2} \quad (|\epsilon| > u)\,. \tag{6}$$

As we can see here the direction of orbital magnetic moment depends on the valley and the directions of the K and K' valleys are opposite to each other.

In the presence of magnetic field $\mathbf{B} = B\hat{\mathbf{e}}_z$ the orbital magnetic moment yields energy shift in the band energy:

$$\epsilon_s \;\to\; \epsilon_s + U_{M\tau}\,, \tag{7}$$

where $U_{M\tau}$ is a Zeeman-like (or, valley Zeeman) energy [23,37] defined as

$$U_{M\tau} = -\boldsymbol{\mathcal{M}}_\tau \cdot \mathbf{B} = \tau U_M\,, \quad U_M = \mu_B^* B\, f(\epsilon, u). \tag{8}$$

Evidently, the energy shift is either positive or negative, depending on the valley. As we shall show below this valley-dependent Zeeman effect plays an important role in the transmission through a BLG junction, leading to valley filtering.

We remark here two points. First, the effective Bohr magneton is much larger than that of real spin: with given values of γ_1 and v_F the effective mass is $m^* \approx 0.032 m_e$, and hence $\mu_B^* \approx 31\mu_B$. It is thus safe to neglect the effect of real spin in the range of magnetic field of interest ($B \lesssim 4$ T, see below) [38]. Second, from Eq. (6), the energy function $f(\epsilon, u)$ has maximum value $f_{max} = 1$ when $\epsilon = s\sqrt{2}u$. Thus, there exists a maximum value of valley Zeeman energy:

$$U_M^{max} = \mu_B^* B \quad \text{when} \quad \epsilon = s\sqrt{2}\,u \tag{9}$$

In what follows, we will use this energy to maximize the valley Zeeman effect on the transmission through a junction.

3. Valley filtration

To investigate the effect of orbital magnetic moment on the transmission we consider both *npn* (barrier) and *pnp* (well) junctions with magnetic filed in the central regions (see Fig. 1). In the present work we assume that the width of sample (the y direction) is large enough so that the edge effects due to boundary conditions can be neglected [39,40]. We choose Landau gauge

$$\mathbf{A}(x) = \left[Bx\Theta(d^2/4 - x^2) \pm \frac{Bd}{2}\Theta(\pm x - d/2)\right]\hat{\mathbf{e}}_y\,, \tag{10}$$

where $\Theta(x)$ is the Heaviside step function and the double signs are in the same order. This choice produces $\mathbf{B} = \nabla \times \mathbf{A} = B\Theta(d^2/4 - x^2)\,\hat{\mathbf{e}}_z$ (perpendicular to the layer) and preserves the translational invariance along the y direction. The Hamiltonian, including the valley Zeeman energy, is then expressed as

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0(B) + V(x) + U_{M\tau} \tag{11}$$

where $\hat{\mathcal{H}}_0(B)$ is given in Eq. (1) with the substitution

$$p_y \;\to\; \pi_y(x) = p_y + eA(x) \tag{12}$$

and the potential is expressed as $V(x) = sV_0\Theta(d^2/4 - x^2)$ with $s = +$ for barrier (*npn*) and $s = -$ for well (*pnp*) and d being the width of potential barrier/well.

The valley filtration can be viewed by writing the wave equation as follows:

$$\hat{\mathcal{H}}_0(B)|\psi(\boldsymbol{r})\rangle = [\epsilon_\tau - V(x)]\,|\psi(\boldsymbol{r})\rangle\,, \tag{13}$$

where $\boldsymbol{r} = (x, y)$ and ϵ_τ is an effective energy incorporating the valley Zeeman term:

$$\epsilon_\tau = \epsilon - \tau U_M\,. \tag{14}$$

Let us consider the *npn* junction, the potential barrier [see Fig. 1(a)]. Outside the barrier (regions I and III), since $V(x) = 0$ and $B = 0$, the energy is an incident energy ϵ. Inside the barrier (region II), however, it becomes effective energy ϵ_τ due to the valley Zeeman term. Now, when the incident energy ϵ coincides with band edge such that $\epsilon = V_0 - u$, the valley-dependent effective energies become $\epsilon_K = V_0 - u - U_M$ and $\epsilon_{K'} = V_0 - u + U_M$, so that ϵ_K lies within the band (the negative energy states) whereas $\epsilon_{K'}$ enters the band gap where no allowed states exist: the K-valley particles are in the Klein tunneling regime and the K'-valley particles undergo ordinary tunneling [41]. As a consequence, the transmission of K'-valley particles will be suppressed, resulting in filtration of the K'-valley particles. The situation is reversed in the *pnp* junction, the potential well. In this case, we have $\epsilon_K = -V_0 + u - U_M$ and $\epsilon_{K'} = -V_0 + u + U_M$, so that the K-valley energy enters the band gap and the K'-valley remains within the band (the positive energy states) [see Fig. 1(b)]. Thus, the *pnp* junction filters off the K-valley particles, while transmitting the K'-valley particles.

To see the valley filtration explicitly, we solve the wave equation (13) numerically by using the method of transfer matrix (see Appendix A for details). As mentioned in Sec. 2 we specialize the case $\epsilon = s\sqrt{2}u$ to maximize the valley Zeeman effect. For the band edge transmission, using the relation $\epsilon = s(V_0 - u) = s\sqrt{2}u$, the incident energy and band gap can be parameterized with potential height/depth V_0: $\epsilon = s(2 - \sqrt{2})^{1/2}V_0$ and $u = (\sqrt{2} - 1)^{1/2}V_0$.

Due to cyclotron motion particles inside the barrier/well will follow curved paths. This restricts the allowed range of magnetic

Please cite this article in press as: C.-S. Park, Valley filtering due to orbital magnetic moment in bilayer graphene, Phys. Lett. A (2017), https://doi.org/10.1016/j.physleta.2017.10.044