Topological zero-line mode of bilayer graphene with Rashba spin-orbital coupling and staggered sublattice potentials

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Domain wall in bilayer graphene with Rashba spin-orbital coupling and staggered sublattice potentials, at the interface between two domains with different gated voltages, is studied. Varying type of zero-line modes are identified, including zero-line mode with pure spin filtering effect. The Y-shape current partition at the junction among three different domains are proposed.

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I. INTRODUCTION

Bilayer graphene (BLG) has tunable band gap that can be controlled by the gate voltage. When gated voltages of opposite signs are applied on the left and right domains of the BLG, the zero-line modes (ZLMs) that are localized near to the interface and exponentially decaying away from the interface are presented. The dispersions are chiral, i.e. the group velocities at K and K’ valley are opposite to each other. Current partition among four ZLMs at a junction has been discussed.

With the present of sufficiently large Rashba spin-orbital coupling (SOC), the gated BLG become topological insulator. The present of staggered sublattice potentials at top and/or bottom graphene layer changes the phase diagram significantly. There are four phases, which are the quantum spin Hall (QSH) phase with topological invariant, top graphene layers respectively; ZLMs, the imaginary part of k-wave solution into the eigen equation gives the Hamiltonian as

where \( \hat{p} = -i\hbar v_F(\tau \partial_x - i \partial_y) \) and \( \hat{p}^+ = -i\hbar v_F(\tau \partial_x + i \partial_y) \) with \( v_F = c_0/330 \) being the Fermi velocity of graphene, \( c_0 \) being the speed of light; \( t_\perp = 0.39eV \) is the inter-layer hopping term between two overlapping carbons, one from the top and the other from the bottom layers; \( \Delta_1 \) and \( \Delta_2 \) are the staggered sublattice potentials for bottom and top graphene layers respectively; \( V(x) \) is the potential difference induced by the gated voltage; \( \tau = \pm 1 \) for K and K’ valleys respectively. The zigzag edge is along the y axis with \( x = 0 \). A kink potential at \( x = 0 \) with \( V(x \geq 0) \) being constant are used throughout this paper. The smooth step-like potential induces additional edge modes near to the bulk band edge, but the ZLMs remain robust.

In this paper, ZLMs of the gated BLG with Rashba SOC and staggered sublattice potentials along the zigzag edge are studied. The gated voltages of two adjoining domains are not necessarily opposite to each other. Rich phases of the topological ZLMs are identified. A new current partition scheme is proposed. In section II, the ZLMs with the absence of the Rashba SOC is reviewed and extended to the case with staggered sublattice potentials. In section III, the ZLMs with the present of the Rashba SOC are studied. The ZLMs in two BLGs with and without staggered sublattice potentials are shown as examples. In section IV, we proposed a scheme of Y-shape current partition. In section V, the conclusion is given.

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relations only depend on $V^2$, $V(x < 0)$ and $V(x > 0)$ have different magnitude in our study, therefore $k_x$ for each domain needs to be calculated separately. With a given pair of $\varepsilon$ and $k_y$, and the corresponding $k_x$, the normalized spinor $\chi$ is obtained, either analytically or numerically, by finding the null space of the matrix $H_A - \varepsilon I$ with $I$ being four by four unit matrix. Among the four solutions of $k_x$, only two of them with proper sign of imaginary part is chosen for each domain. Thus, the wave functions for $x > 0$ and $x < 0$ domain are

$$|\Psi\rangle^\varepsilon = (u_1^\varepsilon \chi_1^\varepsilon e^{ik_2\varepsilon x} + u_2^\varepsilon \chi_2^\varepsilon e^{ik_2\varepsilon x})e^{ik_y}$$  \hspace{1cm} (2)$$

At $x = 0$, all four components of the wave functions are continuous, giving four matching equations for the four unknown constants $u_1^\varepsilon, u_2^\varepsilon$. The ZLMs are found by searching the pairs of $\varepsilon$ and $k_y$ that the determinant of the coefficient matrix of the matching equations being zero. With $\Delta_1 = \Delta_2 = 0$, the ZLMs have been given in the previous publication \cite{2}.

Numerical results of three types of ZLMs are presented in Fig. 1. The ZLMs in suspended BLGs in figure (a) is the same as known. We consider the stagger lattice potential induced by SiC substrate\cite{24}. For the BLGs with $\Delta_1 = \Delta_2 = \Delta = 130meV$, the bulk gap is close at $V = \Delta$, and open with $2\Delta$ at $V = 0$. With the gated voltage being $V = 468meV$, the bulk gap is also $2\Delta$. We studied the ZLMs at the domain wall with $V = 0(V = 468meV)$ at the left(right) domain. Figure (b) shows that the bulk bands of two domains are different, but with the same gap. The dispersion of the ZLMs is nearly linear for a wide range of energy. For the BLGs with $\Delta_1 = -\Delta_2 = 130meV$ in figure (c), the particle-hole symmetry is broken, so that the band structure is not symmetric about $\varepsilon = 0$. All presented ZLMs are in the K valley. The band structure of the corresponding ZLMs in the K' valley can be obtained by mirror reflection $k_y \rightarrow -k_y$ of that in the K valley.

### III. BLGS WITH RASHBA SOC

With the Rashba SOC, the Hamiltonian becomes\cite{26-29}

$$H = \begin{bmatrix} H_A & H_R \\ H_R^* & H_A \end{bmatrix}$$  \hspace{1cm} (3)$$

where

$$H_R = i\hbar\Omega_R \begin{bmatrix} 0 & -\tau + 1 & 0 & 0 \\ -\tau - 1 & 0 & 0 & 0 \\ 0 & 0 & -\tau + 1 & 0 \\ 0 & 0 & -\tau - 1 & 0 \end{bmatrix}$$  \hspace{1cm} (4)$$

and $\hbar\Omega_R$ is the strength of the Rashba SOC. The plane wave solution is spinor having eight components, $|\psi\rangle_R = \chi_R e^{ik_x x + ik_y}$, with $\chi_R = [\chi_A, \chi_B, \chi_A^\varepsilon, \chi_B^\varepsilon, \chi_A^\varepsilon, \chi_B^\varepsilon, \chi_A^\varepsilon, \chi_B^\varepsilon]^T$, where the arrows stand for spin up and down. The relation between $k_x^2$ and $\varepsilon$ is a quartic equation, whose analytical solution is too lengthy to be written in the paper. According to the same principle described in the last section, four solutions of $k_x$ out of eight with proper sign of the imaginary part are chosen for each domain. The wave function for each domain is a superposition of four plane waves, which is similar to Eq. (2). The matching condition at $x = 0$ gives a system of eight linear equations. The ZLMs are found by searching for the pairs of $\varepsilon$ and $k_y$ that corresponding to the zero point of the determinant of the coefficient matrix.

We firstly investigate the ZLMs in the suspended BLG. The results with $V(x \geq 0) = \pm V$ are shown in Fig. 2. When the strength of Rashba SOC is small, the system is in the trivial insulator phase. The SOC splits each ZLM into two bands as shown in Fig. 2(a-d). The dispersions of ZLMs are chiral, meaning that the group velocities in the K and K’ valley are opposite to each other, and the spin expectation in K and K’ valley have the same sign. It can be seen by comparing each thin line of the first column with the thin line of the same style of the third column in Fig. 2. The results of sufficient large strength of the Rashba SOC ($\hbar\Omega_R = 336meV$) is shown in Fig. 2(e-h), where the BLG is driven into the topological insulator phase. For the two ZLMs being plotted as black(solid) and green(dash-dot) lines, the dispersions are chiral with the spin expectation in K and K’ valley having the same sign, which is similar to the ZLMs in trivial insulator. For the other two ZLMs being plotted as red(dotted) and blue(dashed) lines, the spin expectation in K and K’ valley are opposite to each other. The later two ZLMs are originated from the band inversion of the bulk band of the topological insulator.

Secondly, we study the BLGs with substrates being $\Delta_1 = \Delta_2 = 130meV$. The phase diagram is plotted in Fig. 3 in the space of $\hbar\Omega_R$ and $V$. We are particularly interested in the BLGs with $\hbar\Omega_R = 252meV$ and $V$ being one of 546meV, 310meV and 43meV. The three systems, which are marked respectively by dot, circle and square.
All of these four bands are trivial chiral bands. The band structure and spin expectation of the ZLM-III are plotted in Fig. 4(i-l). The band structure and spin expectation of the ZLM-II are at the domain wall between two topological trivial insulators with trivial and non-trivial insulators. ZLM-III is at the domain wall between any two of them supports a ZLM. We denote the ZLM at the domain wall between QSH and QVH as ZLM-I, that between QSH and BI as ZLM-II, and that between QVH and BI as ZLM-III. The band structure and spin expectation of the ZLM-I are plotted in Fig. 4(a-d). There is only one band with nearly perfectly linear dispersion. The dispersions are chiral. At the same energy level, the spin expectation in K and K’ valley are opposite to each other. Thus, the elastic inter-valley back scattering of the ZLM is completely forbidden. The ZLM-I supports pure spin filtering effect.

The current partition scheme at a suspended BLG with V switching sign requires even number of ZLMs at the junction$$[10–14]$$. We show in the following that a Y-shape current partition is possible when staggered potentials and Rashba SOC are involved.

IV. Y-SHAPE CURRENT PARTITION

The current partition scheme at a suspended BLG with V switching sign requires even number of ZLMs at the junction$$[11,14]$$.
drive the BLG into three different topological phases as shown in Fig. 3. Thus, the junction of three phases allows current partition among three ZLMs, as shown in Fig. 5. The group velocity of one ZLM in K and K’ valleys are plotted in Fig. 5(a) and (b), respectively. Assuming the absence of inter-valley scattering, the incident current from the ZLM-III is partitioned into ZLM-I and ZLM-II, as shown in Fig. 5(a). On the other hand, the incident current from the ZLM-I or ZLM-II is redirected to ZLM-III, without current partition as shown in Fig. 5(b). The Y-shape junction induces small inter-valley scattering, producing small back scattering into the incident ZLM. In addition, due to the difference of number of channels, as well as the difference of the wave number and transverse wave functions of the three ZLMs, the transmission coefficients from the import ZLM to the output ZLMs are not integer and the current partition is not evenly distributed.

The proposed scheme for current partition is confirmed by calculations of transportation based on the Landauer-Buettiker formalism and recursively constructed Green’s functions of the tight binding model[30–34]. The conductance between two leads is numerically calculated from the Green’s functions of the scattering region, \( \Gamma \), respectively. For the non-partition current, conductance between two leads is calculated as

\[
G_{ij} = \frac{2e^2}{h} \int dE [t_{ij} G^< (r_j, r_i) - t_{ji} G^< (r_i, r_j)]
\]

where \( r_i \) is the position of the i-th lattice site, \( \hat{d}_{ij} \) is the unit vector from the i-th to j-th lattice site, \( e \) is the electron charge, \( h \) is the Planck constant, \( t_{ij} \) is the hopping parameter between the i-th and j-th lattice site, and \( G^< (r_i, r_j) \) is the lesser Green’s function. The currents through the cross section \( (y_{-1}, y_0) \) and \( (y_0, y_{+1}) \) as a function of x coordinate are defined as \( I_- = \int_{y_{-1}}^{y_0} j_x dy \) and \( I_+ = \int_{y_0}^{y_{+1}} j_x dy \). The 2D spatial distributions of \( j_x \) and the cross section currents are plotted in Fig. 6(a,b), (c,d) and (e,f) with imports from the ZLM-I, ZLM-II and ZLM-III, respectively. At the import side, the incident current are evenly distribute into \( I_- \) and \( I_+ \). The spatially asymmetric reflection at the Y-shape junction, \( I_- \) and \( I_+ \) at the import side are different from each other. With import from the ZLM-I, the reflection is suppressed as shown in Fig. 6(a) and (b), because of the pure spin filtering effect of the ZLM-I. At the output side, the current is redirect into \( I_- \) or \( I_+ \) in Fig. 6(b) or (d), respectively; the current is partitioned into \( I_- \) and \( I_+ \), unevenly in Fig. 6(f). These phenomenons agree with the partition rule of the Y-shape junction. The to-
tal cross section current $I_- + I_+$ remains constant due to the charge conservation.

V. CONCLUSION

In summary, the ZLMs in the BLGs with Rashba SOC and staggered sublattice potentials are investigated. The domain wall between two regions with different gated voltages supports localized chiral edge modes with varying numbers of channels. Particular ZLM with only one channel exhibiting nearly perfectly linear dispersion and pure spin filtering effect is identified. Diversified ZLMs with different dispersions and spin expectation can be obtained by engineering the domain wall between different topological phases. As an example, for the BLGs with $\Delta_1 = \Delta_2$ and fixed $\hbar \Omega_R$, tuning the gated voltage into three values drives the BLGs into three different topological phases with the same band gap. It is shown that the Y-shape junction of the three different topological phases with odd number of domain walls is allowed. The current partition rule at the Y-shape junction is investigated. The diversified ZLMs and Y-shape current partition could boost the development of integrated opto-spintronic and valleytronic devices.

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References

[1] Eduardo V. Castro, K. S. Novoselov, S. V. Morozov, N. M. R. Peres, J. M. B. Lopes dos Santos, Johan Nilsson, F. Guinea, A. K. Geim, and A. H. Castro Neto, Phys. Rev. Lett. 99, 216802 (2007).
[2] Ivar Martin, Ya. M. Blanter, and A. F. Morpurgo, Phys. Rev. Lett. 100, 036804 (2008).
[3] Matthew Killi, Si Wu, and Arun Paramekanti, Phys. Rev. Lett. 107, 086801 (2011).
[4] M. Zarenia, J. M. Pereira, Jr., G. A. Farias, and F. M. Peeters, Phys. Rev. B 84, 125451 (2011).
[5] Jelena Klinovaja, Gerson J. Ferreira, and Daniel Loss, Phys. Rev. B 86, 235416 (2012).
[6] Abolhassan Vaezi, Yufeng Liang, Darryl H. Ngai, Li Yang, and Eun-Ah Kim, Phys. Rev. X 3, 021018 (2013).
[7] Fan Zhang, Allan H. MacDonald and Eugene J. Mele, PNAS, 110(26), 10546-10551 (2013).
[8] Xintao Bi, Jeil Jung, and Zhenhua Qiao, Phys. Rev. B 92, 235421 (2015).
[9] Chaohong Lee, Gun Kim, Jeil Jung, and Hongki Min, Phys. Rev. B 94, 125438 (2016).
[10] Zhenhua Qiao, Jeil Jung, Qian Niu, and Allan H. MacDonald, Nano Lett., 2011, 11 (8), 3453C3459 (2011).
[11] Zhenhua Qiao, Jeil Jung, Chungwei Lin, YaFei Ren, Allan H. MacDonald, and Qian Niu, Phys. Rev. Lett. 112, 206601 (2014).
[12] J. R. Anglin and A. Schulz, Phys. Rev. B 95, 045430 (2017).
[13] Ke Wang, YaFei Ren, Xinzhou Deng, Shengyuan A. Yang, Jeil Jung, and Zhenhua Qiao, Phys. Rev. B 95, 245420 (2017).
[14] YaFei Ren, Junjie Zeng, Ke Wang, Fuming Xu, and Zhenhua Qiao, Phys. Rev. B 95, 245420 (2017).
[15] Hongki Min, J. E. Hill, N. A. Sinitsyn, B. R. Sahu, Leonard Kleinman, and A. H. MacDonald, Phys. Rev. B, 74, 165310 (2006).
[16] Fufang Xu, BaoLei Li, Hui Pan and Jia-Lin Zhu, Phys. Rev. B, 75, 085431 (2007).
[17] Mahdi Zarea and Nancy Sandler, Phys. Rev. B, 79, 165442 (2009).
[18] Emmanuel I. Rashba, Phys. Rev. B, 79, 161409 (2009).
[19] Zhenhua Qiao, Shengyuan A. Yang, Wanxiang Feng, Wang-Kong Tse, Jun Ding, Yugui Yao, Jian Wang and Qian Niu, Phys. Rev. B, 82, 161414 (2010).
[20] Herman Santos, A. Latge, J. E. Alvarelles, and Leonor Chico, Phys. Rev. B, 93, 165424 (2016).
[21] Zhenhua Qiao, Wang-Kong Tse, Hua Jiang, Yugui Yao, and Qian Niu, Phys. Rev. Lett. 107, 256801 (2011).
[22] Zhenhua Qiao, Xiaol Li, Wang-Kong Tse, Hua Jiang, Yugui Yao, and Qian Niu, Phys. Rev. B 87, 125405 (2013).
[23] Xuechao Zhai and Guojun Jin, Phys. Rev. B 93, 205427 (2016).
[24] Ma Luo and Zhibing Li, Phys. Rev. X 3, 021018 (2013).
[25] S. Y. Zhou, G.-H. Gweon, A. V. Fedorov, P. N. First, W. A. de Heer, D.-H. Lee, F. Guinea, A. H. Castro Neto, and A. Lanzara, Nat. Mater. 6, 770 (2007).
[26] Julien Rioux and Guido Burkard, Phys. Rev. B, 90, 035420 (2014).
[27] M. Inglot, V. K. Dugaev, E. Ya. Sherman, and J. Barnas, Phys. Rev. B, 89, 155411 (2014).
[28] M. Inglot, V. K. Dugaev, E. Ya. Sherman, and J. Barnas, Phys. Rev. B, 91, 195428 (2015).
[29] Ma Luo and Zhibing Li, Phys. Rev. B 96, 165424 (2017).
[30] M P Lopez Sancho, J M Lopez Sancho and J Rubio, Phys. F: Met. Phys., 14, 1205-1215 (2014).
[31] Marco Buongiorno Nardelli, Phys. Rev. B, 75, 085431 (2007).
[32] G. S. Diniz, A. Latg, and S. E. Ulloa, Phys. Rev. Lett. 108, 126601 (2012).
[33] Caio H. Lewenkopf, Eduardo R. Mucciolo, J. Comput.
Electron., 12, 203C231(2013).