

Spin electronic manipulation based on zigzag-edge graphene nanojunction with a line defect

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Abstract. We investigate the transport of spin electron through the zigzag-edge graphene nanojunction with a line defect. When the magnetization is zero, the conductance spectra exhibits a well-defined insulating band around the point far away from Dirac point. And the width of the insulating band is exactly equal to the energy splitting between the lowest conduction band of the left lead and the new state of the device region. For the parallel configuration, with the enhancement of the magnetization, the conductance value will be reduced by half around the Dirac point. For the antiparallel configuration, the width of the well-defined insulating band becomes larger with the rising of the magnetization.

1. Introduction

Graphene is the first experimental realization of truly two-dimensional crystal[1], which have exhibited many unusual physical properties in comparison with the conventional semiconductor materials[2,3], rendering it attractive for use in electronics. And the long spin relaxation times[4,5] and the small spin-orbit coupling, further promoting graphene as an interesting material for spintronics applications[2, 6]. Meanwhile, the spin injection from ferromagnetic (FM) metal contacts into graphene has been experimentally achieved[7,8]. The studies have predicted that the spin-polarized carriers can be realized by growing the graphene on a FM insulator[9], others have reported spin current injection in graphene using dynamical and thermal methods[10,11], the nonlocal magneto-resistance measurements have performed, and the graphene-based spin-valve device could have a high magnetoresistance[12,13], so the graphene have attracted a lot of attentions in spin-based quantum computing and spintronics applications. The experimental discovery a peculiar topological line defect in graphene, which can be created by alternating the Stone-Thrower-Wales defect and divacancies[14], extensive attention has been given to this field. The first-principles calculation and experimental observations show that this line defect acts as a one dimensional metallic wire, which motivates researchers to further discuss the electron properties or design the schemes of valley polarization [14,15].

Inspired by possible potential device applications, in this work, based on the Landauer-Buttiker formula and the tight binding model, we investigate the transport of spin electron through the zigzag-edge graphene nanojunctions (ZGNJs) with a line defect.



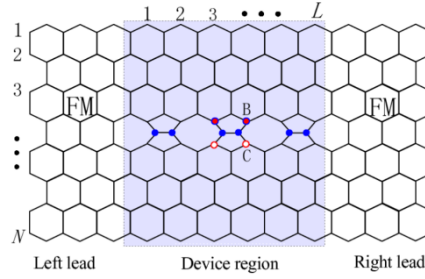


Figure 1. The schematic of the ZGNJs with a line defect.

2. Model and theory

The structure of graphene nanoribbon with zigzag-edge is depicted in figure 1, the structure has three regions: the two semi-infinite FM graphene nanoribbons at the left and the right sides serve as two leads for electronic transmission, which are needed to characterize a clear junction. The central region with a line defect constitutes the device region (shaded), where the electron tunneling is scattered. We use the parameters N and L as the latitudinal and longitudinal size, respectively. We adopt the tight-binding Hamiltonian with nearest-neighbor in-plane interaction to describe the low-energy electronic properties of the graphene nanoribbons. In the tight binding approximation, the single layer of graphene can be described by the following Hamiltonian:

$$H_T = H_d + H_\alpha + H_T \quad (1)$$

the first term H_d is the tight-binding Hamiltonian of the π band electron in the device region.

$$H_C = \sum_i d_i^\dagger (\varepsilon_\alpha \sigma_I + \sigma \cdot M_\alpha) d_i + t \sum_{\langle i,j \rangle} (d_i^\dagger \sigma_I d_j + H.c) \quad (2)$$

where $d_{is}^\dagger$ (d_{is}) is the electron creation(annihilation) operator associated with spin on the local atomic orbits i in graphene, and $d_{is}^+ = (d_{i\uparrow}^+, d_{i\downarrow}^+)$. The notation $\langle i,j \rangle$ means that the summation is restricted between the pairs of the nearest neighbor carbon atoms. t is the corresponding hopping energy. The second term H_α is the Hamiltonian of the two semiinfinite leads.

$$H_\alpha = \sum_i d_i^\dagger (\varepsilon_\alpha \sigma_I + \sigma \cdot M_\alpha) d_i + t \sum_{\langle i,j \rangle} (d_i^\dagger \sigma_I d_j + H.c) \quad (3)$$

$\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and I is a 2×2 unit matrix. ε_d , ε_L and ε_R are the on-site energies in the center region, left and right leads, respectively. M_L and M_R are the magnetizations of the left and right FM leads, which can be along arbitrary direction. The magnetization value in the left and right FM leads are assumed to be equal $M_L = M_R = M$. The last term H_T in the Hamiltonian describes the electron tunneling between the leads and graphene.

$$H_T = t \sum_{\langle i,j \rangle (i \in C, j \in \alpha)} (d_i^\dagger \sigma_I d_j + H.c) \quad (4)$$

with the help of the Landauer-Butikker formula in the discrete lattice representation[16], the linear conductance $\mathcal{G}(E)$ as a function of the incident electron energy E can be evaluated. It gives

$$\mathcal{G}(E) = \frac{e^2}{h} \text{Tr}(\Gamma_L G^r \Gamma_R G^a) \quad (5)$$

where G^r is a retarded Green function, $\Gamma_{L(R)}$ is the coupling function. ε_M is the on-site energies of the line defect. We define the magneto-resistance as $R_M = (\mathcal{G}_P - \mathcal{G}_A) / \mathcal{G}_P \times 100\%$, where $\mathcal{G}_P$ and $\mathcal{G}_A$ are the conductances of the parallel and antiparallel configurations, respectively.

3. Results and discussion

Following the above theory, in the numerical calculation, we will select a unified constant t as the corresponding hopping energy, the lattice constant a is used as the units of the length, the zero point of the energies as the Fermi energy level. When the magnetization $M = 0$, in figure 2 we plot the conductance spectra (G vs E) for the ZGNJs. First, we fixed the width of $N = 12$ and the center region longitudinal size $L=20$ of the ZGNJs. And applying the gate bias ε_d to the device region. The gate bias can be simulated by shifting the on-site energy of all the lattice points. We can see that the conductance drops to zero and presents a well-defined insulating band in the vicinity of the Dirac point. And with the rising of ε_d further, the width of the well-defined insulating band becomes larger. In this regard, we can give an explanation by the sub-band selective rule[17]. Briefly the energy-band of the ZGNJs on the up and down side of the Fermi surface is symmetric and comply with sub-band selective rule, or the electrons belonging to the even (odd) parity subbands in the left ZGNJs are transported only into the even (odd) parity subbands of the right ZGNJs. In addition, we can see that the conductance zero gradually disappear when the ε_d becomes very larger. However when we only change the on-site energy ε_m of the line defect, from the figure 2 we can see that the conductance value remains no change ($G=2 e^2/h$) in the vicinity of the Dirac point. But the width of the conductance valley gradually narrows with the rising of ε_m at the point far away from Dirac point. We can infer that the conductance insulating band arises from the linear defect, which leads to a new zero conductance at the point far away from Dirac point.

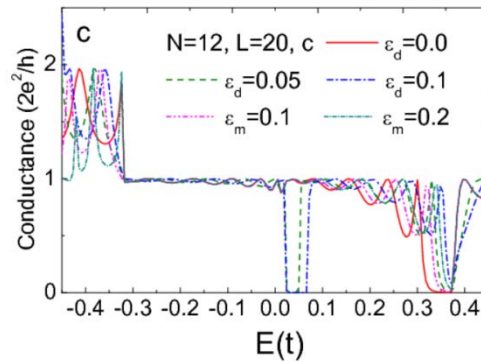


Figure 2. The comparison of the conductance spectra of the ZGNJs, nc representative does not contain line defect, and c represent contains line defect. Change the on-site energy ε_d and ε_m .

In order to further study the influence of the line defect on the conductance spectra of the system, we plot the sub-band structures of the pristine ZGNJs ($N = 12$, nc) and the ZGNJs with a line defect ($N = 12$, c). For a charge neutral junction, from the figure 3, we can see that the Dirac points of the two ribbons are aligned with each other, and two additional states (red line) are included in contrast to the band structure of the pristine ZGNJs. Here we use Δ to label the energy splitting between the lowest conduction band and the Fermi energy of the left lead. And use Δ_m to denote the new state of the device region above the Fermi energy. From the figure 3(b) we also can find that the new state could be tuned by the on-site energy "m of the line defect. Comparing with the conductance spectrum (show in figure 2), we can see that the width of the well-defined insulating band at the point far away from Dirac point is exactly equal to the energy splitting $|\Delta - \Delta_m|$. Accordingly, we found a theoretical explanation that the on-site energy of the line defect can change the width of the well-defined insulating band.

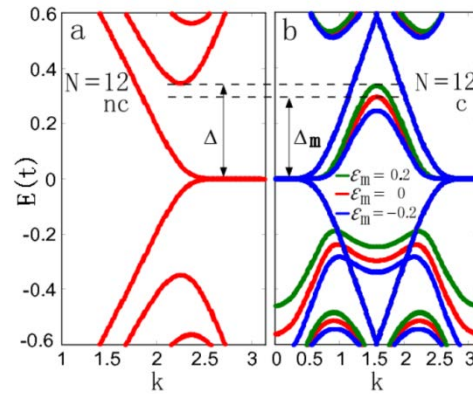


Figure 3. [(a) and (b)] The sub-band structures of the pristine ZGNJs and the ZGNJs with a line defect. Δ and Δ_m denote the energy splitting.

In figure 4(a) and (b), we plot the conductance spectrum of the magnetization $M \neq 0$. In this way we can observe the spin valve effect in the ZGNJs with a line defect. According to the energy band structure of the pristine ZGNJs, we can calculate the energy splitting Δ between the lowest conduction band and the Fermi energy $E_F = 0$, where $\Delta = 0.34$ and $\Delta = 0.27$ for $N=12$ and $N=16$, respectively. In this work, we focus on the conductance behavior in the low-energy region. This is because at this level range, only the lowest electronic conductance channels are involved in electron transport. Therefore, we consider only the case of $M < \Delta$. In addition, for the direction of magnetization, we only consider the parallel $\theta = 0$ and antiparallel $\theta = \pi$ configurations. Firstly, in the parallel configuration, the results show in the figure 4(a). We can see that the conductance value decreased from $G = 2e^2/h$ to $G = e^2/h$ with the enhancement of M in the Dirac point. But the conductance insulating band gradually disappears at the point far away from Dirac point. Secondly, for the antiparallel configuration, from the figure 4(b), we can see that the conductance value decreased from $G = 2e^2/h$ to $G = 0$ in the vicinity of the Dirac point and generating the conductance insulating band, and the width of insulating band becomes larger with the rising of the magnetization M . At the same time, we also can find that the width of insulating band becomes larger at the point far away from Dirac point. Similarly, when we change the size of the central region, we also can find the same conclusion, which suggests that the impact of the magnetization is universal to the conductance spectra.

For these characteristics of the conductance when the magnetization $M \neq 0$, we can give explanation according to the energy band structure. Firstly, for the parallel configurations, the zigzag-edge energy band structure will split and no longer degenerate together with the enhancement of M , which will cause the spin-up electrons and the spin-down electrons have only a single electron conductive channel, respectively. So the conductance value decreased from $G = 2e^2/h$ to $G = e^2/h$ in the vicinity of the Dirac point. Similarly, the splitting can make the energy difference between the lowest conduction band of the left lead and the new state (red line) of the device region decrease. Furthermore it can cause the conductance insulating band gradually disappear at the point far away from Dirac point. Secondly, for the antiparallel configurations, the energy band of the spin-up and the spin-down electrons in the left and the right lead will split along the opposite direction with the enhancement of M , according to the band-selective rule, the spin-up electrons and the spin-down electrons in the center region is no electron conductive channel when the incident electron energy around the Dirac point. Which make the conductance value decreased from $G = 2e^2/h$ to $G = 0$ in the Dirac point and at the point far away from Dirac point.

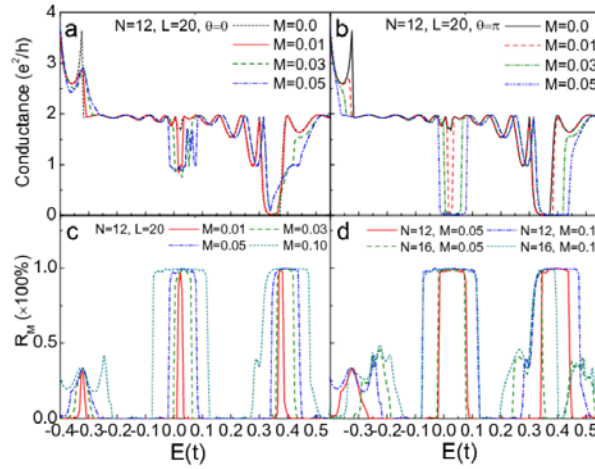


Figure 4. [(a) and (b)] A comparison of the conductance spectrum in parallel configuration and in antiparallel configuration, respectively. (c) The magneto-resistance R_M for different the magnetization M . (d) A comparison of the magneto-resistance by changed the width N and the magnetization M .

Based on the conductances of the parallel and antiparallel configurations, we can plot the magneto resistance R_M as a function of the incident electron energy E for different magnetization M . From the figure 4(c) we can see that the magneto-resistance is very large as far as $R_M = 100\%$ at the Dirac point and at the point far away from Dirac point. In this work, we define the $R_M = 100\%$ as the unit magneto-resistance (UMR). Firstly, by contrast with the band structure, we can find that the width of the UMR at the Dirac point exactly equal to $2M$, and these results for the pristine ZGNJs are also suitable. Secondly, when we fixed the magnetization M and change the width N of the ZGNJs ($N=12$ and $N=16$), from the figure 4(d) we can see that the width of the UMR remains unchanged around the Dirac point. But for the UMR at the point far away from Dirac point, we can see that the plateau width becomes narrow with the increase of the width N . Similarly, when we fixed the width N and change the magnetization M ($M=0.05$ and $M=0.1$), we can find that the width of the two UMR increases with the enhancement of the magnetization M . Meanwhile, we also find the width of the UMR is not affected by the longitudinal size L . By comparing conclusions of figure 4(a) and (b), we can easily find the UMR is derived from the zero conductance in antiparallel configurations. It is worth noting that the plateau width of the UMR (at the point far away from Dirac point) is determined by magnetization M and the size of the center region N . This indicates that it can be considered as a promising candidate for realizing the spin electron transport manipulation.

4. Conclusion

In this work, we have performed a theoretical investigation about the spin electronic manipulation based on ZGNJs with a line defect. The results show that the conductance spectra present a well-defined insulating band at the point far away from Dirac point when the magnetization $M=0$. We find that the width of the insulating band is exactly equal to the energy splitting $|\Delta - \Delta_m|$, and the width of the insulating band could be tuned by the onsite energy ε_m of the line defect. For the parallel configurations, with the enhancement of M , the conductance value decreased from $2e^2/h$ to e^2/h around the Dirac point, and the insulating band gradually disappears at the point far away from Dirac point because of the energy band splitting. For the antiparallel configuration, the band-selective rule makes the width of the insulating band becomes larger with the rising of the magnetization. Based on

the above results, we can find that the magneto-resistance is very large as far as 100%. Compared with the energy band structure, we find that the plateau width of the UMR at the Dirac point is exactly equal to $2M$. And find the plateau width can be readily tuned by the magnetization M and the size N .

Acknowledgments

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