Spin-dependent transport induced by magnetization in zigzag graphene nanoribbons coupled to one-dimensional leads*

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We study spin transport in a zigzag graphene nanoribbon sample with two ferromagnetic strips deposited on the two sides of the ribbon. A tight-binding Hamiltonian was adopted to describe the sample connected to two one-dimensional leads. Our theoretical study shows that the resonance peaks of conductance for the spin-up and spin-down electrons are separated for the parallel configuration of the ferromagnetic strips, while they are not separated for the case of antiparallel configuration. This means that giant magnetoresistance can be produced at particular energies by altering the configurations of the ferromagnetic strips, and the device can be designed as a spin filter.

Keywords: graphene nanoribbon, giant magnetoresistance, conductance, current–voltage characteristic

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1. Introduction

The discovery of giant magnetoresistance (GMR) in 1988[1] has led to a rapid development in spintronics, which exploits the intrinsic spins of electrons in transport phenomena. Much attention has been paid to the study of spin-based devices recently due to their attractive advantages, such as faster data-processing speeds and lower electric power consumption. Graphene, a single atomic layer of carbon with low intrinsic spin–orbit and hyperfine couplings[2] and a long spin diffusion length,[3] has opened up a new area for spintronics. Graphene nanoribbons (GNRs) with zigzag edges can be made to carry spin currents under external fields,[4] which may enable a new region to explore spintronics at the nanoscale. A spin-effect transistor has been proposed by utilizing a graphene layer as the channel, where the spin manipulation is achieved.[5] It was shown that when a single B or N atom was doped in the central region of the zigzag graphene nanoribbons (ZGNRs), the spin-polarized current could be generated.[6] Hwang *et al.* predicted a negative magnetoresistance for intrinsic graphene and found a non-monotonic magnetoresistance for extrinsic graphene under a parallel magnetic field.[7] A new type of magnetoresistive device has been proposed, which makes use of the remarkable electronic properties of the ZGNRs.[8] Zhang *et al.* also proposed an alternative system to realize the spin polarization and the GMR, which contains a ZGNR sample with two ferromagnetic strips deposited on the two sides of the graphene ribbon.[9]

Most of the studies on the transport properties of graphene are based on two-dimensional graphene electrodes.[6,8,9] The electrodes can be constructed by different dimensionality electronic systems. Li *et al.* demonstrated that the dimensionality of metal contacts had a strong effect on the current–voltage (I–V) characteristics of the molecular junctions.[10] Likewise, research on the transport properties of graphene should also consider the effect of the dimensionality of the leads. More recently, Zhou *et al.* investigated the spin-dependent transport properties of the armchair-edge graphene nanoribbons with three-dimensional ferromagnetic electrodes, and many new phenomena were revealed.[11] The electron transport properties of the GNRs connected to one-dimensional leads have also attracted much attention.[12−14] From the experimental point of view, such research makes sense when

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the graphene couples to the probes of the scanning tunneling microscope[15] or the ultrathin gold or tungsten wires. It can therefore be anticipated that the spin-dependent transport properties of GNRs coupled to one-dimensional leads are worth studying.

Motivated by the above discussion, in this paper we study spin polarization and the GMR effect induced by magnetization in a ZGNR sample connected to two one-dimensional leads. Our proposed system is similar to that given in Ref. [9], except for the leads. Figure 1 shows a GNR with a zigzag edge in the (x, y) plane. Two ferromagnetic stripes are deposited on two sides of the ribbon. Two semi-infinite one-dimensional electrodes – source and drain – are attached to the two extreme ends of the graphene to maintain the uniformity of the quantum interference effects. The directions of magnetization of the ferromagnetic stripes can be parallel or antiparallel, and can be tuned by a magnetic field. Using the nonequilibrium Green's function (NEGF) method, the conductance–energy (G–E) and the I–V characteristics can be obtained by numerical calculations. The results indicate that the conductance spectra show sharp resonance peaks mainly due to the mismatch of the interfaces between the graphene and the leads. The resonance peaks of conductance for the spin-up and the spin-down electrons are separated only at the parallel configuration of the ferromagnetic strips. Hence, GMR can be produced for particular energies in the system, and the present device can be designed as a spin filter at the parallel configuration.

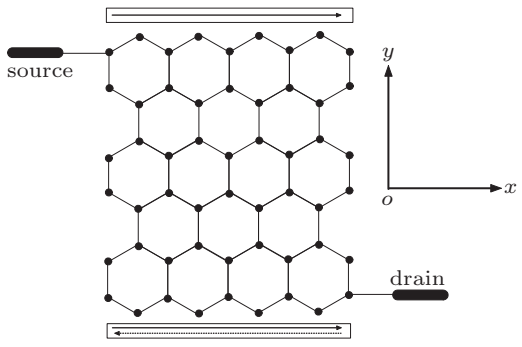


Fig. 1. Schematic diagram of the system. Two ferromagnetic stripes are deposited on the top and down sides of the GNR, and source and drain leads are attached to the two extreme ends of the graphene.

2. Model and methods

Based on the tight-binding model, the Hamiltonian of the graphene can be described as[9]

$$H = \sum_{i,\sigma}(\varepsilon_i + \lambda_\sigma W_i)c^\dagger_{i,\sigma}c_{i,\sigma} + t\sum_{\langle i,j\rangle,\sigma}(c^\dagger_{i,\sigma}c_{j,\sigma} + \text{H.c.}), \quad (1)$$

where ε_i is the site energy, $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator of an electron at site i with spin σ ($\sigma = \uparrow, \downarrow$), $\lambda_\sigma = \pm 1$ for $\sigma = \uparrow, \downarrow$, t is the nearest neighbour hopping integral, and W is the magnetization induced in the graphene by the two ferromagnetic strips attached to the two sides of the graphene ribbon. Under the antiparallel configuration of the ferromagnetic stripes, the magnetization decreases gradually from W to $-W$ from one side of the graphene to the other along the y direction. Under the parallel configuration, the magnetization reaches the maximum value of W at the two sides and gradually decreases to zero in the middle of the graphene. A similar kind of tight-binding Hamiltonian is also used to describe the two semi-infinite one-dimensional perfect electrodes, where the Hamiltonian is parameterized by constant on-site potential ϵ_0 and the nearest neighbour hopping integral t_0.

Using the Landauer conductance formula, the conductance G_σ of the graphene with spin σ in the linear transport regime can be expressed in the form

$$G_\sigma = \frac{e^2}{h}T_\sigma, \quad (2)$$

where e is the charge of an electron, h is the Planck constant, and T_σ is the transmission probability of an electron with spin σ in the ribbon. It can be obtained from[16]

$$T_\sigma = \text{Tr}[\Gamma^\sigma_{\text{S}} G^{r,\sigma}\Gamma^\sigma_{\text{D}} G^{a,\sigma}], \quad (3)$$

where $G^{r,\sigma}$ and $G^{a,\sigma}$ are the retarded and the advanced Green's functions of the ribbon, including the effects of the two electrodes, and can be written as

$$G^{r,\sigma} = (G^{a,\sigma})^\dagger = (E + \text{i}\,\eta - H_\sigma - \Sigma^\sigma_{\text{S}} - \Sigma^\sigma_{\text{D}})^{-1}. \quad (4)$$

Here, E is the injecting energy of the source electron, $i\eta$ is a small imaginary term added to make the Green's function non-hermitian, and Σ^σ_{S} and Σ^σ_{D} are the self-energies due to the two electrodes and can be analyzed through the use of Newns–Anderson chemisorption theory.[17] The Γ^σ_{S} and Γ^σ_{D} are the coupling matrices, which represent the couplings of the graphene to the source and drain, respectively. They are defined by the relation

$$\Gamma^\sigma_{\text{S(D)}} = \text{i}[\Sigma^\sigma_{\text{S(D)}} - (\Sigma^\sigma_{\text{S(D)}})^\dagger]. \quad (5)$$

The current with spin σ passing through the ribbon can be computed as a function of the applied bias voltage V through the relation

$$I_\sigma(V) = \frac{e}{h}\int_{-\infty}^{+\infty}[f_{\rm S}(E) - f_{\rm D}(E)]T_\sigma(E)\,{\rm d}E, \quad (6)$$

where $f_{\rm S(D)}(E) = f(E-\mu_{\rm S(D)})$ gives the Fermi distribution function of the source (drain) electrode having a chemical potential of $\mu_{\rm S(D)} = E_{\rm F} \pm eV/2$, and $E_{\rm F}$ is the equilibrium Fermi energy. Here we make a realistic assumption that the entire voltage is dropped across the ribbon–electrode interfaces. It is found that under such an assumption, the I–V characteristics do not change their qualitative features.[13]

3. Results and discussion

In the following numerical calculations we set the site energies of the graphene as $\varepsilon_i = 0$ for all i, as we concentrate only on the cleaned systems. The nearest-neighbour hopping integral t in the graphene is set to 2, and the on-site energy ϵ_0 and hopping integral t_0 for the two electrodes are fixed to 0 and 2, respectively. The hopping strengths of the graphene to the source and drain are set at $\tau_{\rm S} = \tau_{\rm D} = 1.5$. Compared with the effect of the self-energies to the transport properties of the graphene, the thermal effect can be neglected.[13] Accordingly, we can set the temperature to zero in the following calculations. We take the magnetization to be $W = 0.1t$.[9] The graphene is composed of many hexagons and is described with width N and length M. Parameter M determines the number of hexagons in each row, while N determines the number of rows of hexagons. Following this rule, a graphene with $N = 3$ and $M = 4$ corresponds to three rows of hexagons attached side by side, and each row contains four hexagons (see Fig. 1). The following numerical results correspond to the graphene with $N = 3$ and $M = 6$. For the sake of simplicity, we choose the unit with $h = c = e = 1$.

First, the conductance G ($G = G_\uparrow + G_\downarrow$) as a function of injecting energy E for the two configurations of ferromagnetic stripes is illustrated in Fig. 2. The conductance spectra show resonance peaks for some particular energies, which is similar to the results in Ref. [10]. On account of the one-dimensional leads, this is largely due to the mismatch of the interfaces between the leads and the graphene. For the anti-parallel configuration, the number of resonance peaks is smaller, and some of the peaks have heights close to 2. While for the parallel configuration, there are more resonance peaks, and most of the peaks do not have heights exceeding 1. The reason for this is that the resonance peaks for the spin-up and the spin-down electrons are separated in the parallel configuration, while they are not separated in the anti-parallel configuration. For different configurations, the distributions of the resonance peaks are different. This means that the GMR can be achieved for the present system in the energy areas where the resonance peaks appear.

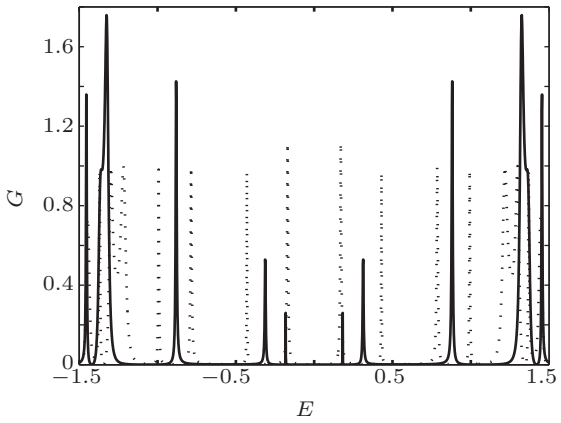


Fig. 2. Conductance, G, as a function of injecting electron energy, E, where the solid and dotted curves correspond to the results for the anti-parallel and parallel configurations, respectively.

As mentioned above, the conductance resonance peaks for the spin-up ($G_\uparrow$) and spin-down ($G_\downarrow$) electrons are separated at the parallel configuration, which is shown in Fig. 3. The spin-up and spin-down electrons have different channels while passing through the graphene. The spin-up channels are symmetrical to the spin-down channels about the zero energy point. Moreover, most of the channels have

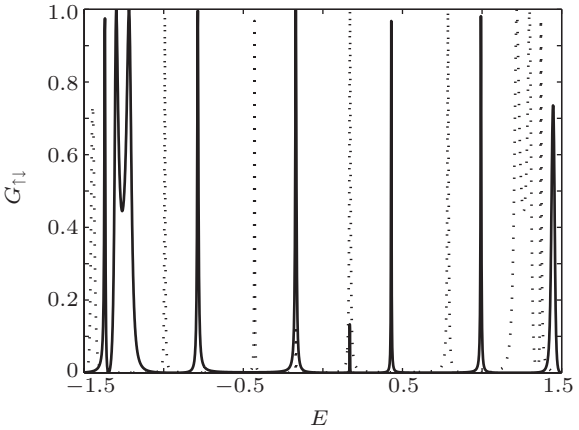


Fig. 3. Spin-dependent conductance, $G_{\uparrow\downarrow}$, as a function of energy, E, for parallel magnetization, where the solid (dotted) curve is for spin-up (spin-down) electrons.

the maximum transmission probability. Interestingly, we can also find continuous conduct energy areas for the spin-up and spin-down electrons, such as the areas around $E = -1.25$ for the spin-up electrons and around $E = 1.25$ for the spin-down electrons. These behaviours indicate that the present device at the parallel configuration can work as a spin filter.

The spin filter action becomes clearer in the I–V characteristics shown in Fig. 4. The current with spin σ passing through the graphene can be obtained from Eq. (6), and is determined from the integration procedure of the transmission function. With the increase in bias voltage, V, the electrochemical potentials of the two leads cross one of the resonance peaks of the graphene, and accordingly an obvious increase in the I–V curve appears. Thus, the currents passing through the graphene exhibit a step-like behaviour. In Fig. 4 we set the value of $E_{\rm F}$ at -1.25. Around this value of $E_{\rm F}$, only conductance resonance peaks for the spin-up electrons exist (see Fig. 3). Hence, when the bias voltage is in the region of about -0.3 to 0.3, a pure spin-up current is obtained, and the spin-down current is totally blocked. In a similar way, if we set $E_{\rm F}$ at 1.25, a pure spin-down current can be obtained.

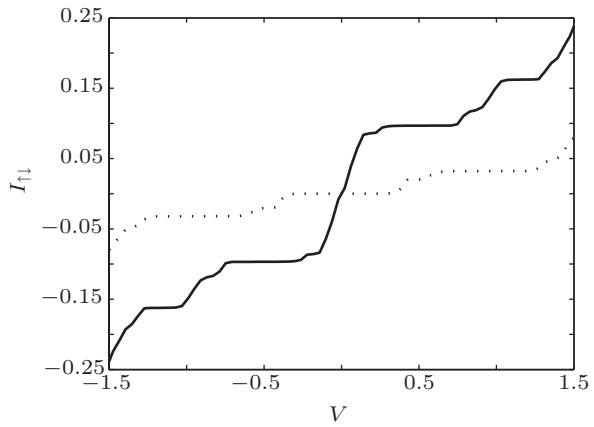


Fig. 4. Current, $I_{\uparrow\downarrow}$, as a function of bias voltage, V, in a parallel configuration with $E_{\rm F} = -1.25$. The solid and dotted curves correspond to spin-up and spin-down electrons, respectively.

4. Conclusion

In summary, spin transport through a ZGNR was theoretically studied using the NEGF formalism. We adopted the tight-binding framework to illustrate the system, which is a GNR modulated by configurations of the ferromagnetic strips and connected to two one-dimensional leads. For the parallel configuration, the resonance peaks of conductance for spin-up and spin-down electrons were separated, while they were not separated at the antiparallel configuration. A huge GMR can thus be achieved in the graphene device. Due to the separation of the conduction channels for different spin electrons, the GNR at the parallel configuration can be designed as a spin filter. We also gave the I–V characteristics of the system to demonstrate the spin filtering action. It was found that pure spin-up and pure spin-down currents can be obtained up to a threshold bias voltage.

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