Spin-polarized transport in a normal/ferromagnetic/normal zigzag graphene nanoribbon junction*

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We investigate the spin-dependent electron transport in single and double normal/ferromagnetic/normal zigzag graphene nanoribbon (NG/FG/NG) junctions. The ferromagnetism in the FG region originates from the spontaneous magnetization of the zigzag graphene nanoribbon. It is shown that when the zigzag-chain number of the ribbon is even and only a single transverse mode is actived, the single NG/FG/NG junction can act as a spin polarizer and/or a spin analyzer because of the valley selection rule and the spin-exchange field in the FG, while the double NG/FG/NG/FG/NG junction exhibits a quantum switching effect, in which the on and the off states switch rapidly by varying the cross angle between two FG magnetizations. Our findings may shed light on the application of magnetized graphene nanoribbons to spintronics devices.

Keywords: spontaneous magnetization, zigzag graphene nanoribbon, spin polarizer, quantum switching effect

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1. Introduction

The graphene nanoribbon, a strip of graphene, has recently received much attention, because it is not only a building block of future graphene electronic devices but also exhibits very extraordinary properties,[1−13] e.g., the zero-energy edge state forms in the quasi-one-dimensional zigzag graphene nanoribbon (ZGNR), the spontaneous magnetization[2] is found at the edge atoms of the ribbon. Density functional calculations[3,4] indicate that the ground state of a ZGNR is an antiferromagnetic (AFM) band insulator, that is, the spontaneous magnetizations on the two edges are antiparallel to each other, while keeping ferromagnetic ordering along the two edges of the ribbon. The ferromagnetic (FM) ZGNR has also been investigated extensively by numerical calculations[3−6] and found to be metallic. Moreover, the energy difference between the AFM and the FM states in a unit cell is fairly small and decreases rapidly with the increase of the zigzag-chain number N. Therefore, an FM ZGNR could be easily stabilized by applying an experimentally accessible magnetic field or using a supporting FM insulator.[11]

In addition to the spontaneous magnetization in the ZGNR, the peculiar current-blocking effect or the valley-valve effect[14−18] is also found in the ZGNR p–n junction. This phenomenon can be accounted for by the so-called valley selection rule. The wavefunction of a particle at the K or K' valley has a definite pseudoparity. The transmission of a particle in a p–n junction is allowed only when the injected and the transmitted particles have the same pseudoparities; therefore, the current-blocking effect is present in an even ZGNR but absent in an odd ZGNR. Currently, information about the combined effect of the spin transport from the spontaneous magnetization and the valley selection rule in ZGNRs is lacking, although some nanoscale spintronic devices built around the phenomenon of spin polarization have been proposed in the literature.[5−8]

2. Model and method

In this work, we study the spin-dependent electron transport in single and double nor-

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mal/ferromagnetic/normal (NG/FG/NG) ZGNR junctions by considering the interplay between the edge magnetization and the valley-selection rule. In our previous work,[19] we have shown that the ferromagnetism in a ZGNR can stem from the spontaneous magnetization due to the Coulomb interaction, and can be stabilized by mounting a ferromagnetic insulator,[19] doping,[20] hydrogenation,[21,22] etc. Such intrinsic magnetization is vitally important, because it does not destroy the structural symmetry of the ZGNR or the pseudoparity of the particle. Whereas due to the extrinsic magnetization from an FM metal deposited on a ZGNR, it is difficult to keep the pseudoparity of the ZGNR unchanged in reality. By using the lattice Green's method, we calculate the conductance of the junction and find that in the NG/FG/NG junction, only one spin-species current is allowed to flow whereas the other spin-species current is entirely prohibited due to the valley-selection rule, so the single NG/FG/NG can act as a spin polarizer and/or a spin analyzer; while the double junction NG/FG/NG/FG/NG can behave as a perfect quantum switch, in which the on and the off states switch rapidly by changing the cross angle between the two FG magnetizations.

We start with the NG/FG/NG junction shown schematic in Fig. 1(a), where the ZGNR connects the source and the drain electrodes, the FG segment is stabilized by an FM insulator, and the magnetization mainly resides on the edge atoms. The length of the FG segment is La, and the zigzag-chain number of the ZGNR is N, where $a = 2.46$ Å is the lattice constant of the graphene. It is noticed that the FM insulator is not a unique choice to stabilize the FG, any alternative[11,20] that can make the FM state more stable than the AFM state is feasible, as long as it does not destroy the pseudoparity of the ZGNR. For instance, a semihydrogenated ZGNR[21] was demonstrated to be in the FM state and kept the structural symmetry unchanged. The following Hamiltonian is employed to describe the junction:

$$H = -t \sum_{\langle ij\sigma \rangle} (C^{\dagger}_{i\sigma} C_{j\sigma} + \text{c.c.}) + U \sum_{i\sigma} (n^{\dagger}_{i\sigma} n_{i\bar{\sigma}}), \quad (1)$$

where $C^{\dagger}_{i\sigma}$ ($C_{i\sigma}$) is the creation (annihilation) operator at site i with spin σ ($\sigma = \uparrow\downarrow$), $\bar{\sigma} = -\sigma$, $\langle ij \rangle$ denotes the nearest-neighbour sites, t is the hopping integral, the last term refers to the on-site Coulomb interaction with U being the Coulomb constant, and $n_{i\sigma}$ is the σ-spin electron number operator at site i.

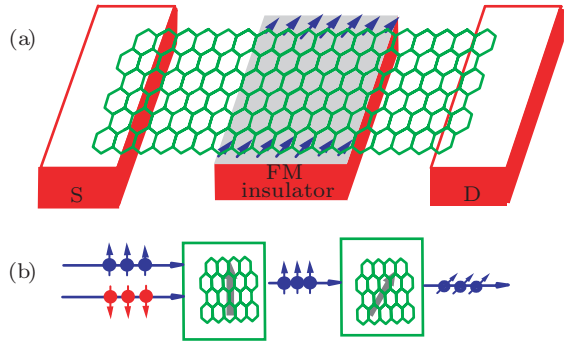


Fig. 1. (colour online) (a) Schematic of the NG/FG/NG junction with spontaneous FM magnetization, which mainly resides at edge atoms of the ribbon and is stabilized by an FM insulator. (b) Spin-filter and spin-analyzer device made from the single NG/FG/NG junction, unpolarized electrons are incident into the first junction, with only one spin-species electron allowed to pass. Meanwhile, such transmitted spins can be detected by the second junction with a different FG magnetization direction.

The Hartree–Fock approximation is adopted here to deal with the Coulomb interaction, and the FM structure in a uniform ZGNR can be obtained by assuming an initial FM distribution in the ZGNR for self-consistent calculation, as done in Ref. [19]. The spin density $\langle n_{i\uparrow} - n_{i\downarrow} \rangle$ distribution in a unit cell of the FG region is assumed to decrease linearly to zero in the NG region. The spin-dependent conductance $G_{\sigma\sigma'}$ is given by

$$G_{\sigma\sigma'} = \frac{e^2}{h} \text{Tr}[\Gamma_{\text{L}\sigma} g^{\text{r}}_{\sigma\sigma'} \Gamma_{\text{R}\sigma'} (g^{\text{r}}_{\sigma\sigma'})^{\dagger}], \quad (2)$$

where g^{r} is the retarded Green's function of the junction, and $\Gamma_{\text{L(R)}\sigma}$ is the σ-spin line-width function of the left (right) NG. The g^{r} can be calculated by using direct matrix inverse $g^{\text{r}} = [E - H_{\text{c}} - \Sigma_{\text{L}} - \Sigma_{\text{R}}]^{-1}$, where H_{c} is the effective single electron Hamiltonian of the FG segment under the Hartree–Fock approximation, and $\Sigma_{\text{L(R)}}$ is the self-energy of the left (right) NG lead. Actually, a recursive method is adopted to evaluate the retarded Green's function g^{r}. The $G_{\sigma\sigma'}/(e^2/h)$ is the transmission coefficient of the particle from the left σ-spin channel to the right σ'-spin channel. The total conductance of the junction is given by $G_{\text{T}} = \sum_{\sigma\sigma'} G_{\sigma\sigma'}$.

3. Numerical result and discussion

In this section, we calculate the spin-dependent electron transport in the single and the double

NG/FG/NG junctions according to the formula introduced in the previous section. In our calculations, the FM magnetization direction is set to be the spin quantum axis of the system, the hopping energy is $t = 2.8$ eV, the Coulomb constant[3,4] is $U = 1.3t$, and the width of the ribbon is $N = 20$. The spin-resolved electron occupation $\langle n_{i\sigma}\rangle$ on each site of the FM ZGNR can be worked out within the Hartree–Fock approximation, and the obtained spin density[19] at the edge atom of the FG is $n_\uparrow - n_\downarrow \simeq 0.32$. It is assumed that the spin density decreases linearly to zero from the FG region to the NG region[a)] in the following discussion.

In Fig. 2, the spin-resolved conductance $G_{\uparrow(\downarrow)}$ of the single NG/FG/NG junction is presented as a function of the Fermi energy $E_{\rm F}$. It is shown clearly that when only a single transverse mode (the edge state) contributes to the current, the spin-up channel is open whereas the spin-down channel is closed if $E < E_{\rm F}$, the situation is reversed if $E > E_{\rm F}$, and the total conductance remains one quantum conductance $G_{\rm T} = G_\uparrow + G_\downarrow = e^2/h$ in the single-mode transport regime. This originates from the valley selection rule, since the spin-dependent p–n–p or n–p–n junction always exists for one of the spin channels wherever the Fermi energy is taken to be, and the corresponding spin channel is closed. In other words, the single NG/FG/NG junction is actually a spin-filtering device,[12,13] since only one spin-species particle can pass through such a junction whereas the opposite spin-species particle cannot.

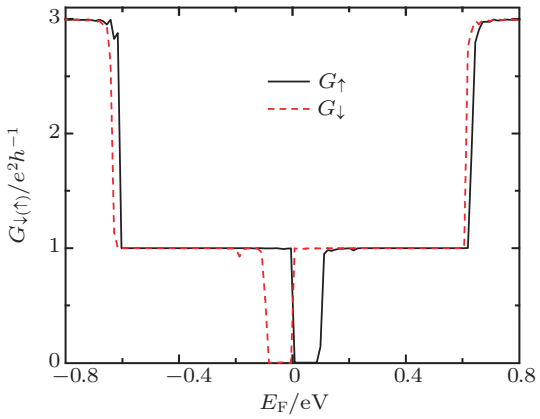


Fig. 2. (colour online) Variation of spin-polarized conductance of the NG/FG/NG junction with Fermi energy $E_{\rm F}$, with parameters being $N = 20$ and $L = 100$.

In order to better understand the above phenomenon, we plot the spin-dependent band structures of normal graphene and FM graphene around the band centre, as shown in Fig. 3. It is seen in Fig. 3(b) that the magnetization can lift the spin degeneration. The symmetries (pseudoparities) of the bands are denoted by different line styles: the solid lines represent σ symmetry, with which the wave functions exhibit even parity; the dotted ones denote C_2 symmetry, with which the wave functions exhibit odd parity.[12,13] Due to the parity conservation of the transverse wave function and the band-selection rule,[23] only electrons having the same parities as those of the wave functions in the FM region can pass through the device. Thus, only the spin-down electrons can contribute to the current when the Fermi energy is above zero, and the ZGNR is an insulator for the spin-up electrons in this case. The situation is exactly opposite when $E_{\rm F}$ is below zero. In this latter case, the spin-up electrons have the same orbital parities in the normal and the FM regions, so they can flow through the device, while the conductance for the spin-down channel is now zero.

Similarly, the single NG/FG/NG junction can also act as a good spin analyzer. When a spin with an arbitrary direction $\boldsymbol{n}(\theta, \phi)$ is incident into the junction, the transmission coefficient through the junction should be proportional to $\cos^2\frac{\theta}{2}$ or $\sin^2\frac{\theta}{2}$, which is dependent on the filtering spin state $(1,0)^{\rm T}$ or $(0,1)^{\rm T}$ of the junction. In other words, when the injected spin is parallel to the filtering spin, it will pass through the junction; otherwise, it will be blocked. Therefore, the NG/FG/NG junction function behaves like an optical polarizer. As shown in Fig. 1(b), the first junction can make unpolarized electrons become fully polarized, while the second junction can detect the spin direction of the transmitted electron.

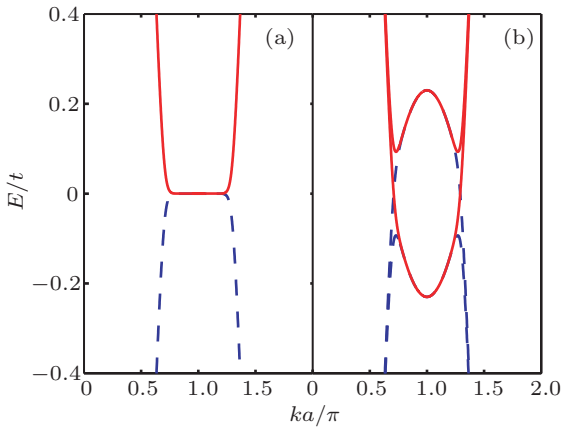


Fig. 3. (colour online) Energy band structures of (a) normal graphene and (b) FM graphene.

We proceed to examine the coherent transport in an NG/FG/NG/FG/NG junction composed of two FG regions, a standard spin-valve structure. In Fig. 4, the conductance $G_{\rm T}$ is calculated as a function of cross

[a)] The length of the transitional region with decreasing spin density is set as $La/10$ between the uniform FG and the NG.

angle θ between the two FG magnetizations. As expected, the total conductance is basically proportional to $\cos^2\frac{\theta}{2}$, and exhibits a clear quantum switching effect between the on ($G_{\rm T}=1$) and the off ($G_{\rm T}=0$) states. Moreover, under appropriate parameters, the transition between on and off is very swift, and the resonant peak of the on/off state is fairly wide, which is related to the chiral nature of the particle in the ZGNR. The relation between the Fermi energy and the magnitude of the spontaneous magnetization can also affect such a swift transition. When the Fermi energy $E_{\rm F}$ approaches the spin-split electron or the hole band edge of the FG segment, the transition between the on and the off states becomes more rapid. As seen in Fig. 4(a), the slope of the $E_{\rm F}=0.092$ eV curve is larger than those of the other two curves. The $E_{\rm F}=\pm0.092$ eV is the energy boundary of the first transverse mode shown in Fig. 2.

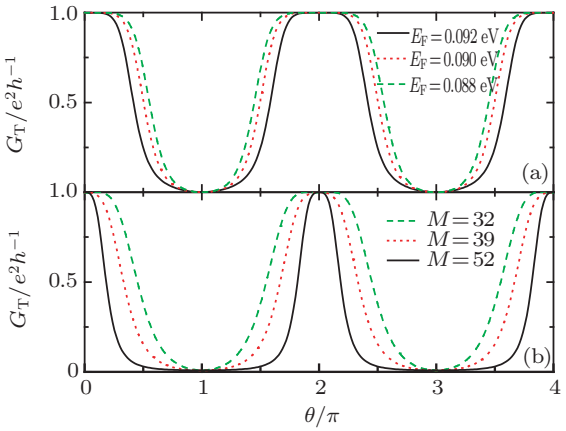


Fig. 4. (colour online) Total conductance of the NG/FG/NG/FG/NG junction as a function of cross angle θ between the two FG magnetizations with (a) different values of Fermi energy $E_{\rm F}$ and (b) different lengths of middle NG layer Ma. Parameters are $M=32$ in (a) and $E_{\rm F}=0.092$ eV in (b).

The findings in Figs. 2 and 4 are not expected to occur in normal FM metal materials such as iron and cobalt. As conventional conducting FM materials are not perfect half-metals, neither of the two spin-specie channels can be closed entirely. As a result, the perfect spin polarizer/detector effect as well as the efficient quantum switching effect will not appear in normal FM junctions or even in armchair GNR junctions. Currently, a nanosize graphene ribbon with zigzag edges has been fabricated in experiment, and even spontaneous edge magnetism has been observed,[24] which can facilitate the implementation of our proposed device. Certainly, the key point to realize such a spin filtering effect and a quantum switching effect is to make a perfect FM-ZGNR segment and keep the C_{2h} symmetry[19] of the system undestroyed, because without the C_{2h} symmetry, the definite pseudoparity of the particle in the ZGNR does not exist, and the valley selection rule is invalid. Therefore, the spontaneous FM magnetization in the ZGNR is desirable, although the magnetization in the ZGNR induced by the lateral FM metal materials,[12,13,25–27] which is assumed not to destroy the C_{2h} symmetry of the ZGNR, can lead to the same spin filtering effect, the anisotropic stray field and the inhomogeneous magnetization from the FM metal can easily destroy the pseudoparity of the particle in the ZGNR in reality.

4. Summary and conclusion

We investigate the spin transport in single and double NG/FG/NG junctions, the FM in the ZGNR comes from the spontaneous magnetization due to the Coulomb interaction. It is shown that the single junction can act as a spin polarizer and/or an analyzer while the double NG/FG/NG/FG/NG junction behaves as a perfect quantum switch. The physics origin results from the valley selection rule in the even ZGNR and the spin splitting in the FG region. Our findings may be useful for fabricating spintronic devices based on graphene nanoribbons.

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