Spin transport through a triangular graphene flake

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Abstract. We theoretically investigate the coherent spin polarized transport through a graphene flake by focusing on the magnetic effect of the zigzag edges. The graphene flake with triangular shape is sandwiched between two nonmagnetic one dimensional electrodes. The semi-infinite electrodes cannot effectively alter the ferromagnetic spin configuration at the zigzag edges. The electronic structure and magnetic properties of this junction are simulated self consistently by use of the single-band tight-binding approximation and the mean-field Hubbard model. Our numerical results show that the spin transport strongly depends on the magnetic configuration of the graphene flake and hence, a fully spin-polarized conductance without external field can be produced. In addition, the current-voltage characteristic shows a high splitting between spin-up and spin-down currents due to the effect of edge-induced magnetism on the electronic transport through the graphene flake. The results may be useful for carbon-based spintronic applications.

1. Introduction
The control and manipulation of spin degree in carbon-based systems have attracted much attention due to experimental possibility to fabrication and the special charge and spin transport properties [1]. In such structures the spin-polarized currents conserved due to the low spin orbit interaction and weak hyperfine coupling [2]. Various experimental and theoretical works are applied to investigate the feasibility of generation of carbon-based spin-dependent device. [3, 4]

The honeycomb lattice of graphene is a bipartite lattice which is formed by two triangular sublattices A and B [5, 6]. For a bipartite lattice and the Hubbard repulsive parameter the imbalance between the total number of atoms in the two sublattices can produce a total spin \(2S = N_A - N_B\) [6]. Also, the zigzag edge of graphene flake at the ground state has an antiferromagnetic spin alignment that is mostly localized at the zigzag edge and has its largest value of the magnetic moment at the edge.

In this paper, we theoretically investigate the spin-polarized transport through a triangular graphene flake sandwiched between two one-dimensional nonmagnetic electrodes which paying special attention to the magnetic effects of atoms in the scattering region. To reduce the effects of electronic structure of the electrodes on the scattering region, we consider the case that only one carbon of the graphene flake is connected to each electrode, as shown in Figure 1(a). The graphene flake which consists of 78 carbon atoms has ferromagnetic spin configuration due to its special design at the zigzag edges.
edges. In this case the three sides of triangular channel belong to the same sublattice and hence, same magnetic moments localized at the edges. The total spin value at the scattering region, according to the Lieb’s theorem, reaches \( S = 3 \) and we found that the semi-infinite electrodes cannot effectively alter this spin configuration.

2. Formalism and Model

Here the Hamiltonian of the left and right one-dimensional electrodes is described within the single-band tight-binding approximation and takes the form

\[
H_\alpha = \sum_i \varepsilon_i d_\alpha^\dagger d_\alpha - t \sum_{ij} d_\alpha^\dagger_i d_\alpha_j
\]

where \( d_\alpha^\dagger \) (\( d_\alpha \)) creates (destroys) an electron at site \( i \) in electrode \( \alpha (=R,L) \), \( t \) is the hopping integral between nearest-neighbor atoms and \( \varepsilon_i \) is the on-site energy of the electrodes. The electron conduction is mainly determined by triangular junction. In order to obtain the magnetic moment of each atom in the scattering region, we use the Hubbard model within the unrestricted Hartree-Fock approximation and tight binding model. Therefore, the central part of the device is described using the mean-field Hubbard model for the \( \pi \) orbitals with nearest neighbor hopping \( t \) and the on-site Coulomb interaction \( U \). Therefore, the channel Hamiltonian can be written as [7,8]

\[
H_C = -t \sum_{\alpha,\sigma} d_{i\alpha}^\dagger d_{i\sigma} + U \sum_i \left( \langle n_i \rangle n_{i\uparrow} \langle n_{i\downarrow} \rangle \right) - \langle n_i \rangle \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle
\]

where \( d_{i\alpha}^\dagger \) (\( d_{i\alpha} \)) creates (annihilates) an electron with spin \( \sigma \) at site \( i \), \( n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma} \) is the number operator and \( \langle n_i \rangle \) denotes the spin-dependent expectation value for the number operator at site \( i \). We solve self consistently the mean field Hamiltonian by an iteration method. Therefore the Green’s function and the spin density on each atom in the channel should be iteratively calculated until a convergence of the charge density is reached. The Green’s function of the graphene flake (channel) is written as [9]

\[
G_C(E,\nu) = [E - H_C - \Sigma_L(E,\nu) - \Sigma_R(E,\nu)]^{-1}
\]

here \( \Sigma_\alpha(E) = -t \exp(ik_\alpha a \cdot \mathbf{R}) \) is the self-energy which contains the influence of the electronic structure of the semi-infinite electrodes on the channel.

Figure 1. (a) The triangular graphene flake with two nonmagnetic one dimensional electrodes (narrow arrows). (b) DOS for the channel in contact with the electrodes. (c) Transmission coefficients as a function of energy at zero gate voltage. The solid (dashed) line is for majority (minority) spin electron.
We assume that the hopping parameter and lattice constant of the electrodes are same as the graphene flake.

Using the equation (3) for the non-equilibrium Green’s function (NEGF), the spin-dependent density of states and the expectation value for the number operator of electron with spin $\sigma$ at site $i$ in the central region, are given by

$$
\rho_\sigma(E) = -\frac{1}{i}\text{Im}\langle i\sigma|G(E)|i\sigma\rangle, \\
\langle n_\sigma\rangle = \int dE\rho_\sigma(E)
$$

The magnetic moment on each carbon atoms can be written as $m_i = (\langle n_{i}\uparrow\rangle - \langle n_{i}\downarrow\rangle)\mu_B$. The transmission probabilities of spin-up and spin-down channels are independent and the electronic transport can be decoupled into two spin currents: one for spin-up and the other for spin-down. Therefore, the spin-dependent currents for a constant bias voltage are calculated by the Landauer-Buttiker formalism [9]:

$$
I_{\sigma}(V_a) = \frac{2e}{h}\int_{-\infty}^{\infty} T_{\sigma}(\varepsilon, V_a) [f(\varepsilon - \mu_{L}) - f(\varepsilon - \mu_{R})]d\varepsilon
$$

where $f(\varepsilon)$ is the Fermi-Dirac distribution function, $\mu_{L,R} = E_F \pm eV_a/2$ are the chemical potentials of the electrodes and $T_{\sigma}(\varepsilon, V_a) = Tr[\hat{G}_\sigma\hat{T}_a\hat{G}_\sigma^\dagger]$ is the spin- energy- and voltage-dependent transmission function. Using $\Sigma_a$, the coupling matrices $\Gamma_a$ can be expressed as $\Gamma_a = -2\text{Im}(\Sigma_a)$

### 3. Result and discussion

We study the results of electronic density of states (DOS), the transmission coefficients, and the current-voltage characteristics. The DOS for the triangular graphene flake has been shown in Figure 1(b). In the figure, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are clear. The complete separation between the majority and the minority electrons in most of the energy ranges explains the localized magnetization at the graphene flake. The interaction between the molecular levels of graphene flak and the surface states of semi infinite electrodes has a week broadening effect on the electronic structure of nanodisk. Therefore, the DOS show sharp peaks as shown in Figure 1(b). In the presence of the electrodes, the difference between two spin-polarized densities of states at each atomic site doesn’t change notably except at the contact sites and the maximum value of the magnetic moment reaches 0.24 $\mu_B$. The Fermi energy shifts from zero to $E_F = 0.94$ eV due to the Hubbard repulsive parameter ($U = 2.82$ eV).

Transport through molecules is different with respect to the bulk materials, i.e., standard metals or semiconductors, due to the collapse of Fermi energy into a single energy level HOMO [10]. The transport properties are mainly determined by HOMO and LUMO levels. In the case of small bias voltage, the probability of transmission for spin-down electrons is more than the spin-up ones. Figure 1(c) shows the transmission coefficients as a function of energy for spin-up and spin-down electrons. We see that the transmission coefficient at zero gate voltage has a number of sharp peaks and spin-down peak appears near the Fermi energy. It is clear that, in most of the energy ranges, the values of transmission are completely separated. This is due to the spin-dependent scattering at the Fermi energy.

We have studied the degree of spin polarization (P) for electrons traversing the channel which can be defined as $P(\varepsilon) = [T_{\uparrow}(\varepsilon) - T_{\downarrow}(\varepsilon)]/[T_{\uparrow}(\varepsilon) + T_{\downarrow}(\varepsilon)]$. From the transmission spectrum it is clear that, we can obtain a spin-polarization as high as 100%. This spin polarization of the electron conduction can play an important role on the spin-dependent transport through the graphene flake. For this reason, we have plotted in Figure 2(a) the spin currents in terms of the applied voltage. From the I-V characteristic, we see the step like behavior for two spin subbands. The minority peak at the Fermi energy is responsible for spin down electron conduction at low bias. Also, the applied voltage can change the difference between both the spin-up and spin-down currents significantly.
The influence of gate voltage shifts the molecular levels relative to the Fermi energy of electrodes, and hence the transmission coefficient may significantly vary [11]. Since the currents depend on the molecular levels laying between the left and right chemical potential, by altering the gate potential the molecular levels shift inside the energy window and the intensity and polarization of current for two spin currents change. To show the effect of gate voltage, we plot the current verses the gate voltage in Figure 2(b). In some ranges of gate voltage there isn’t any peak of DOS and the current verses the gate voltage vanishes.

4. Conclusion
In this work, the coherent spin-polarized transport through triangular junction was investigated based on the non-equilibrium Green’s function technique, and the mean-field Hubbard model. We have shown that the graphene flake whit zigzag edge is strongly spin selective and perfect spin polarization can be produced without applying magnetic field or magnetic materials.

The difference between the transmission coefficients of two spin subbands in most of energy ranges is very large and there is a great spin splitting between two transmission coefficients even in the range of energy which is far from the Fermi energy. Consequently, high spin-polarized currents can be produced. In addition, one can manipulate the degree of spin polarization by applying a gate voltage and a bias potential on the channel and electrodes, respectively. These results may be useful for spin injection into the semiconducting spintronic devices.

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