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Spin related transport in two pyrene and Triphenylene graphene nanodisks using NEGF method

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ABSTRACT

The present study is conducted to evaluate the spin polarization in two pyrene and Triphenylene graphene nanoflakes. All calculations are performed using non-equilibrium Green's function (NEGF) method. The obtained results show that, graphene has no magnetic property and using Pyrene nanoflake results in a better spin switching at extreme magnetic fields. On the contrary, when applying magnetized electrodes, depending on the direction of magnetization of the two electrodes (either parallel or anti-parallel), different spin polarization diagrams are obtained. In this situation, it is observed that, in the case of electrodes magnetization in Triphenylene nanoflake a better spin switching is reached.

1. Introduction

Due to their unique electrical,.optical and mechanical properties, graphene and related structures have been attracted by many researchers [1–4]. Since the discovery of graphene in the laboratory in 2004, many scientists have hoped to use this material with unique properties in the production of electronic devices [5–7]. The lack of band gap in this material makes it difficult to apply it in keying devices. Although limiting this structure in one dimension and producing nanoribbons permits to create a small band gap, it results in a significant decrease in electron mobility. Ideas based on the production of spin transistors based on spin-dependent transmissions by the semiconductor channel have been formed since 1990. The diminishing growth of transistors causes the transistor channel to shrink. Therefore, moving toward the production of transistors with very small channels is inevitable. Spin polarization with unique properties of graphene and its small dimensions motivated us to explore the spin transport from graphene nanoflakes.

The spin transport from the graphene connections was studied by a large number of scientists as an attractive idea [8–11]. Due to the small structure of nanoflakes, evaluation of nanoflakes has an own attraction. Evaluation of the electrical and spinal effects of Pyrene and Triphenylene nanoflakes was performed by Szałowski in 2001 [12]. In his presentation, the lack of characteristics of the voltage-current curve for this structure was obvious, therefore in the present study, it has aimed to examine this structure in the presence of a strong magnetic field to obtain the effect of the current. Moreover, Lii et al. conducted a study to obtain stripe structure and specification of current-voltage from triangular graphene nanoflakes using the computational software in 2016 [13]. Sheng and colleagues obtained the electrical properties of triangle nanoflakes by computational software [14]. Lii and colleagues calculated the current flow through a transistor with graphene nanoflake channel using simulation software. The results showed that, when the nanoflakes were large enough, a spin filter was created spontaneously due to the effects of the edge [15]. But in the case of small nanoflakes, there should be an external factor to separate the spin. Among the conducted calculations, unbalanced Green's approach has been used lesser that other methods to obtain the current - voltage characteristics from the pyrene and Triphenylene nanoflakes. Obtaining a spin filter from the nanostructures can help information-based tools generation based on electron spin. In the present study, graphene nanoflakes were considered as carbon atoms with sp^2 hybrids and an electron in the π orbital perpendicular to the plate responsible for the transfer of charge. In this orbital, two high spin electrons experienced the Coulomb interaction in the Hubbard model. In this study, the effect of this interaction was considered disorderly and up to the first level, which was the Hartree–Fock approximation. In this model, the exchange term was zero and only the Hartree term remained. A strong magnetic field perpendicular to this plate was considered to create a separation in the electron population with opposing spins.

2. Calculations

The present article aimed to consider the graphene nanoflake con-

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nected to one-dimensional electrodes. To stimulate this issue, one-dimensional electrodes were considered as a semi-finite array of quantum dots [16]. In Fig. 1, the studied segment was shown. The Hamiltonian of the entire structure is given as

$$H = \sum_{\alpha_j=L,R} \varepsilon_\alpha \left(a^\dagger_{j,\alpha} a_\alpha\right) + \sum_{\alpha_j=L,R} T_\alpha \left(a_{j+1,\alpha} a^\dagger_{j,\alpha} + a_{j,\alpha} a^\dagger_{j+1,\alpha}\right) + \sum_n \varepsilon_{d_n} {d_n}^\dagger d_n + \sum_{\alpha_n=L,R} t_{n\alpha}\left(a_{1,\alpha} {d_n}^\dagger + d_n a^\dagger_{1,\alpha}\right) + \sum_{i,j=nn} {t'}_{ij}\left(d^\dagger_i d_j + d^\dagger_j d_i\right) \quad (1)$$

In Eq. (1), a and $a^\dagger$ are creation and annihilation operators in electrodes and d and $d^\dagger$ are creation and annihilation operators in quantum point, respectively. The first two terms are Hamiltonian electrodes, which contains the total electron energy of each site and jump energy from one site to another. The third term is the quantum dot Hamiltonian, and the fourth term is the tunneling Hamilton from the electrodes to the quantum dot. The last Hamiltonian term is related to the Hamiltonian nanoflake and n.n means summation on nearest neighbors. T_α is the coefficient of electron hoping in the electrode α. $t_{n\alpha}$ is the hopping term of electron from electrode α to atom n of nanoflake. t'_{ij} is electron jump coefficient from neighbor atoms to each other in nanoflake. The passing current can be calculated using

$$J_\alpha = \frac{2e}{2\pi\hbar}\int d\varepsilon \mathrm{Re}\left[tr\left(G^r_d(\varepsilon)\sum\nolimits^<_L(\varepsilon) + G^<_d(\varepsilon)\sum\nolimits^a_L(\varepsilon)\right)\right] \quad (2)$$

where G is quantum point Green's function and $\sum$ is self-energy. Self-energy is defined in terms of equilibrium Green's functions of electrode as [17].

$$\sum\nolimits^{r,<,a}_{mn}(\varepsilon) = \sum_{\alpha\beta=R,L} \delta_{\alpha\beta} t_{m\alpha} g^{r,<,a}_\alpha(\varepsilon) t_{\beta n} \quad (3)$$

The electron Green' functions are defined as

$$g^<_{\alpha=L,R}(xt,x't') = i\left\langle {\widehat{\Psi}_\alpha}^\dagger(x't')\widehat{\Psi}_\alpha(xt)\right\rangle$$
$$g^r_{\alpha=L,R} = -i\theta(t-t')\left\langle\left\{\widehat{\psi}(\overrightarrow{x},t), \widehat{\psi}^\dagger(\overrightarrow{x}',t')\right\}\right\rangle \quad (4)$$

where $\widehat{\Psi}_\alpha(xt)$ and ${\widehat{\Psi}^\dagger}_\alpha(xt)$ are creation and annihilation operators of the electron. Since the electrodes are considered in the semi-infinite, the electron wave function is in the form of $\psi(x) = \sqrt{2/L}\sin(n\pi x/L)$, which is presented in

$$\widehat{\Psi}_\alpha(xt) = \sum_k \psi_{\alpha k}(x) a_{\alpha k}(t) \quad (5)$$

where a is Fermionic annihilation operator. By calculating Eq. (4), Eqs. (6) and (7) are obtained as

$$g^<_{\alpha=R,L}(\varepsilon) = \frac{-2i}{T_\alpha}\sqrt{1-\left(\frac{\varepsilon-\varepsilon_{0\alpha}}{2T_\alpha}\right)^2} f_\alpha(\varepsilon) \quad (6)$$

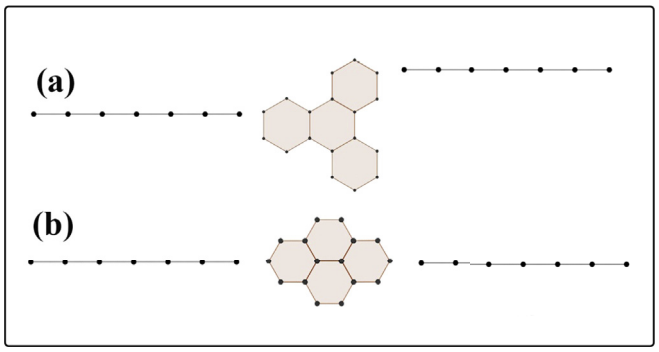

Fig. 1. a) Triphenylene structure; b) Pyrene structure.

$$\mathrm{Re}\left(g^R_\alpha\right) = \frac{1}{T}\left[\left(c_\alpha - \sqrt{{c_\alpha}^2-1}\right)\left(\Theta(c_\alpha-1) - \Theta(-c_\alpha-1)\right)\right]$$
$$\mathrm{Im}\left(g^R_\alpha\right) = \sqrt{1-c^2_\alpha}\Theta(1-|c_\alpha|) \quad (7)$$
$$c_\alpha = \frac{\varepsilon-\varepsilon_{0\alpha}}{2T_\alpha}$$

After obtaining the electrode Green's function, it is possible to calculate the self-energies by Eq. (3). Note that for Green's function we always have [18].

$$G^R(\varepsilon) = \left((\varepsilon+i\eta)\widehat{I} - H_s - \sum\nolimits^R(\varepsilon)\right)^{-1}$$
$$G^A(\varepsilon) = \left(G^R(\varepsilon)\right)^\dagger$$
$$G^<(\varepsilon) = \left(1+G^R(\varepsilon)\times\sum\nolimits^R(\varepsilon)\right)\times G^<_0(\varepsilon)\times\left(1+\sum\nolimits^R(\varepsilon)\times G^a(\varepsilon)\right) + G^R(\varepsilon)\times\sum\nolimits^<(\varepsilon)\times G^a(\varepsilon) \quad (8)$$
$$G^> = G^R + G^< - G^A$$
$$G^<_0 = if_S(E)\mathrm{Im}\left(G^R_0(E)\right)$$

where f *is* the fermionic distribution function. The densities of different states of the system are given by Ref. [16].

$$DOS(\varepsilon) = \frac{-1}{\pi} tr(G^R(\varepsilon)) \quad (9)$$

When the electrons have a Coulomb repulsion interaction with each other at π level, this interaction is described in Hubbard model. This situation should be added to the Hamiltonian of Eq. (1) as

$$V = Un_\uparrow n_\downarrow$$
$$n_{\uparrow(\downarrow)} = d^\dagger_{\uparrow(\downarrow)} d_{\uparrow(\downarrow)} \quad (10)$$

Using high potential and expansion of the Cuban function up to the first level of the disorder results in self-energy of the first level as

$$\sum\nolimits^R_{U\uparrow\uparrow} = -\frac{iU}{2\pi\hbar}\int d\omega\, G_{\downarrow\downarrow}{}^<(\omega)$$
$$\sum\nolimits^<_U(\varepsilon) = 0 \quad (11)$$

Eqs. (11) and (8) can be solved in a self-adaptable manner to obtain the self-energy of electron-electron interaction and finally, total self-energy is obtained by summarizing Eqs. (3) and (11).

3. Results

3.1. Pyrene nanoflakes

The spectrum function of this structure is shown in Fig. 2. The band gap is 5.3 electron volts and the interaction of the electron-electron results in a displacement about U/2 in the sample. In Fig. 3, the spin polarization graph is plotted for this structure. It can be seen that in the voltage gate from zero to 1.5 V, the spin polarization movies from positive to negative. This fact can be considered in spin keying. Moreover, spin polarization is not noticeable in this situation due to the lack of magnetic property in graphene. If the electrodes have magnetic properties, the situation will be different. The effect of the magnetization of the electrodes can be considered in the difference electron jump coefficient with different spin in the Hamiltonian [19]. In this study, two parallel and nonparallel magnetization modes in the electrodes were compared, and the jump coefficient of high spin was 0.02 and the jump coefficient of low spin was 0.01. For parallel and nonparallel mode $t_{L\uparrow} = t_{R\uparrow} = 0.544$ eV; $t_{L\downarrow} = t_{R\downarrow} = 0.272$ eV and $t_{L\uparrow} = t_{R\downarrow} = 0.544$ eV; $t_{L\downarrow} = t_{R\uparrow} = 0.272$ eV were calculated, respectively. The results of parallel and nonparallel magnetization modes for pyrene nanoflake are shown in