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Aharonov-Casher effect and quantum transport in graphene based nano rings: A self-consistent Born approximation

A. Ghaderzadeh [a], S.H. Ebrahimnazhad Rahbari [b], A. Phirouznia [a,c,*]

[a] Department of Physics, Azarbaijan Shahid Madani University, 53714-161 Tabriz, Iran
[b] School of Physics, Korea Institute for Advanced Study, Seoul, South Korea
[c] Condensed Matter Computational Research Lab. & Computational Nanomaterials Research Group (CNRG), Azarbaijan Shahid Madani University, 53714-161 Tabriz, Iran

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ABSTRACT

In this study, Rashba coupling induced Aharonov-Casher effect in a graphene based nano ring is investigated theoretically. The graphene based nano ring is considered as a central device connected to semi-infinite graphene nano ribbons. In the presence of the Rashba spin-orbit interaction, two armchair shaped edge nano ribbons are considered as semi-infinite leads. The non-equilibrium Green's function approach is utilized to obtain the quantum transport characteristics of the system. The relaxation and dephasing mechanisms within the self-consistent Born approximation is scrutinized. The Lopez-Sancho method is also applied to obtain the self-energy of the leads. We unveil that the non-equilibrium current of the system possesses measurable Aharonov-Casher oscillations with respect to the Rashba coupling strength. In addition, we have observed the same oscillations in dilute impurity regimes in which amplitude of the oscillations is shown to be suppressed as a result of the relaxations.

1. Introduction

Beginning of the twenty-first century has witnessed a tremendous exposure of graphene both because of its ample applications in science and technology [1–4]. This establishes graphene as an emerging intensive research field [1]. Noticeably, low energy electrons in graphene appear as relativistic (Dirac) particles which behave like massless Dirac fermions [2]. Interestingly, low energy excitations create most of the intriguing properties of the graphene [5]. Many studies aim at investigation of fundamental properties of graphene [6–8]. Far before its recognition as an extraordinary material, in a pioneering work Wallace formulated the electronic properties of graphene [9].

From the structural point of view, graphene can be regarded as a zero-gap semiconductor or zero-overlap semi-metal [2]. As a one-atom-thick two-dimensional (2D) allotrope of carbon packed in a honeycomb lattice, graphene is considered as a basic building block for other graphitic materials [10,11].

One of the most interesting graphene based structures is the graphene nano ribbons which can be constructed by cutting strips of graphene [12]. The electronic properties of graphene nano ribbons depend on the ribbons width, type of the edge, and the chirality. In Zigzag graphene nano ribbons band structure (ZZ-graphene nano ribbons), the energy gap becomes zero at the edges of the Brillouin zone. Furthermore, in armchair graphene nano ribbons (AC-graphene nano ribbons) the number of dimer lines, N, determines the energy band gap [13].

Revisiting many standard quantum mechanical effects for graphene has been a subject of many studies. The Aharonov-Bohm effect is the modulation of the charge current as a result of the external magnetic field. This effect is theoretically revisited for graphene based quantum rings by Beenakker and Wurm [14,15]. It is also experimentally confirmed by Russo et al. [16]. The Aharonov-Casher (AC) effect can be considered as dual effect of the Aharonov-Bohm (AB) effect. The difference between the AB and the AC effects is that the latter is a consequence of interaction of dipole moment with an external electric field, however, the former appears as a result of electric charge interaction with an external magnetic field.

In this study, the Aharonov-Casher effect has been obtained by the Rashba spin-orbit interaction (RSOI) which arises as a result of an electric gate voltage. The RSOI is a controllable interaction that can be tunably controlled by this gate voltage.

Influence of the spin-orbit interaction in single layer graphene has been described by Kane and Mele [17,18]. Strength of intrinsic spin-orbit coupling (ISOC) in graphene is very small in comparison with the RSOI [19–24]. The Rashba coupling strength in graphene, has been predicted to be up to 0.2 eV [25]. This value can be considered as a relatively high coupling strength for a typical spin-

* Corresponding author at: Department of Physics, Azarbaijan Shahid Madani University, 53714-161 Tabriz, Iran.
E-mail address: Phirouznia@azaruniv.ac.ir (A. Phirouznia).

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orbit interaction. Therefore, it can be expected that the Rashba coupling related effects in graphene will be significantly different from the similar effects that can arise by this interaction in the other two-dimensional structures.

In the current study, we have considered a graphene based nano ring as the central device connected with two semi-infinite armchair leads. We have studied the Aharonov-Casher (AC) effect caused by the Rashba spin-orbit interaction. Influence of the Rashba spin-orbit interaction can be considered as a process in which the spin of the conduction electrons are flipped while hopping to the nearest neighboring atoms [26–28]. This interaction results in oscillation of the electric current as a function of the Rashba coupling which is known as the Aharonov-Casher effect [29,30].

We have employed the nonequilibrium Green's function (NEGF) formalism which is known as the standard approach in the investigation of the quantum transport in mesoscopic systems and molecular electronics [31]. The NEGF provides a microscopic theory for investigation of internal interactions and relaxation mechanisms [32]. In addition, we have utilized the Lopez-Sancho approach [33] for obtaining the self-energy of the lead-device coupling. In this way, we are able to treat the real-space self-energy of the leads. Equipped with the Lopez-Sancho approach, we are able to calculate surface Green's function instead of hopping all lead atoms [5] in a semi-infinite lead within a fast converging numerical approach [33]. Meanwhile the effect of the impurity and lattice vibrations are obtained within the self-consistent Born approximation in which the self-energy of the scattering process have been given in the context of the diagrammatic analysis. Since the lattice vibrations alter the effective hopping amplitude, we have found that the Rashba interaction is modified in the presence of the atomic vibrations. Therefore we have considered the effect of the vibronic couplings at very low Rashba couplings.

We have scrutinized dependence of the electric current oscillations to of the Rashba coupling in pure and impure systems. All above mentioned calculations have been performed for a graphene based Aharonov-Bohm system with a central ring shaped structure containing 114 carbon atoms connected with semi-infinite armchair leads as depicted in Fig. 1.

2. Nonequilibrium Green's function formalism

Perturbative formalism, in most of the cases, is the only approach which could be used to obtain expectation value of an observable in a many-particle system. Nonequilibrium Green's function approach is an important technique which can be applied as a perturbative method especially to obtain the transport properties of open quantum systems [32]. The Green's Function of the system is given by

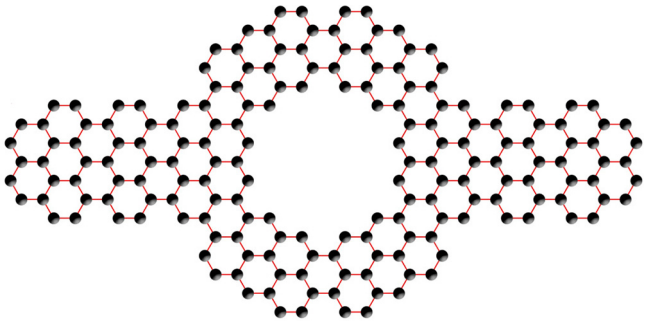

Fig. 1. Graphene nano ring connected to two semi-infinite graphene nano ribbons as leads in Armchair shaped edge.

$$G^{(R/A)}(E) = \lim_{\eta\to 0^+} \frac{1}{E \pm i\eta - H}, \tag{1}$$

where G^R and G^A denote retarded and advanced Green's functions respectively in which $(G^{(R)\dagger}(E) = G^{(A)}(E))$, η is a small positive value and H is the Hamiltonian of the system.

Therefore the full Hamiltonian can be described as

$$\widehat{H} = \widehat{H}_D + \widehat{H}_L + \widehat{H}_P, \tag{2}$$

where $\widehat{H}_D$ is Hamiltonian of the central device, $\widehat{H}_L$ is Hamiltonian of the leads and $\widehat{H}_P$ denotes the interaction of the electrons with disorders which should be treated perturbatively.

In the current system the effective Hamiltonian of the system in tight-binding approximation is as follow

$$H_D = E_0 \sum_i c_i^\dagger c_i - t \sum_{<i,j>} c_i^\dagger c_j + \widehat{H}_R, \tag{3}$$

where $\langle i,j\rangle$ represents the nearest neighbors and $c_i^\dagger(c_i)$ is an operator that creates (annihilates) an electron at site i and t is the nearest neighbor hopping in the graphene where we have assumed $(t \approx 2.7\ \text{eV})$ that fits well with tight-binding approximation. Here it was assumed that the Rashba interaction has been induced by a perpendicular electric field, $E = E\hat{z}$. In this case the Hamiltonian of the Rashba coupling reads [26,27]

$$\widehat{H}_R = it_R \sum_{\langle i,j\rangle} c_i^\dagger \left(s \times \hat{\mathbf{d}}_{ij}\right).\hat{\mathbf{z}} c_j + h.c.. \tag{4}$$

Rashba coupling strength, t_R, depends on the electric field and increases by increasing this external field, s is the vector of Pauli matrices and $\hat{d}_{ij}$ is the unit vector which connects the i and j lattice sites.

The contribution of the leads is given by the sum of the left and right Hamiltonians denoted by the $\hat{H}_L$ as follows

$$\hat{H}_L = \sum_i (\widehat{H}_L^i + V_{LD}^i + V_{DL}^i), \tag{5}$$

in which $i =$ left or right, labels either side of the ring, $\widehat{H}_L^i$ is the Hamiltonian of the i-th lead, V_{LD}^i is the hopping between lead and device and similarly V_{DL}^i is the hopping between device and lead where we have $V_{DL}^i = (V_{LD}^i)^\dagger$ [5]. The Hamiltonian of the leads could be effectively represented by proper self-energies that can be given by

$$\Sigma_i^R = V_{DL}^i g_L^i V_{LD}^i, \tag{6}$$

where Σ_i^R stands for the retarded self-energy of i-th lead, g_L^i is the Green's function of the isolated semi-infinite lead defined as

$$g_L^i = \frac{1}{E + i\eta - H_L^i}. \tag{7}$$

The Lopez-Sancho method [33] is the approach which provides the self-energy of the semi-infinite leads. Meanwhile it has been shown that the only relevant part of the Green's function of the lead in the transport properties of the system is the surface Green's function which has been considered as a Green's function of the coupling region of the Lead-system [5].

3. Aharonov-Casher and Aharonov-Bohm effects

As mentioned before the Aharonov-Casher (AC) effect can be considered as a counterpart of the Aharonov-Bohm effect. Aharonov-Bohm effect could be described by the influence of the magnetic field on the transport of the electric carriers, meanwhile