Physica E 57 (2014) 76–82

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Study of the electron–photon interaction on the spin-dependent transport in nano-structures

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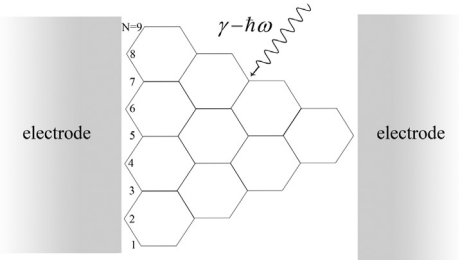
HIGHLIGHTS

- A tight binding study of transport through a triangle quantum dot between two leads.
- Our results show a relatively large spin polarization in the current–voltage curve.
- The spin polarization is controlled in the presence of light illumination.

GRAPHICAL ABSTRACT

We studied the transport through a graphene quantum dot in the presence of light illumination.



ARTICLE INFO

Article history:
Received 28 September 2013
Received in revised form
21 October 2013
Accepted 23 October 2013
Available online 9 November 2013

Keywords:
Graphene quantum dot
Hubbard model
Electron–photon interaction

ABSTRACT

Transport through a nano device in the presence of light illumination has been studied by using unitary-transformation scheme together with the non-equilibrium Green's function formalism. The non-interacting Hamiltonian is written within the framework of the tight binding model and structureless electrodes are described in wide-band approximation. The interaction between electrons is modeled by the mean-field Hubbard term. Our results indicate that we can tune the "intrinsic magnetization of zigzag edge" and "spin-polarized current" by using light illumination.

1. Introduction

The nano science is about the investigation of structure in the molecular scale. The electronic transport through a nano scale device sandwiched between two leads is an interesting topic for both experimental [1–4] and theoretical physicists [5–13]. The non-equilibrium Green's function formalism is an appropriate model for investigation such a transport trough a nano device [5–7,9–13]. In the presence of different many body interactions the transport becomes a sophisticated problem from the theoretical point of view. The electron–electron interactions are very important in the transport properties of nano-devices which are responsible for the Coulomb blockade and the Kondo effect [9,14,15]. The coupling between the fermionic and bosonic systems of such a device is very interesting. Due to the very long spin relaxation and de-coherence time graphene is an appropriate material for future spintronic devices [16,17]. Most of the recent works based on the mean-field theory or configuration interaction (CI) method predict the net magnetic moments in the zigzag edges of graphene quantum dots due to the sub-lattice symmetry breaking [18–24]. In this work, a typical triangle graphene quantum dot (T-GQD) with zigzag edges between two infinite electrodes in the presence of light illumination has been considered. We investigate the electron–photon interaction in a typical nano scale

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http://dx.doi.org/10.1016/j.physe.2013.10.031

device which is an applicable model for photo-detector devices. The electron–electron interactions are modeled by using the mean-field Hubbard Hamiltonian. The dark self-energy which is the self-energy in the dark condition contains the effect of left and right electrodes on the T-GQD. Our main goal is to investigate the effect of the electron–photon interaction on the magnetic and spin-dependent transport properties of nano device considered here. The theoretical investigation of electron–photon interaction provide a better understanding of underlying physics to design more efficient nano-photonic devices. Here, the main problem comes from the coupling between the fermion and boson system. We present two successive methods for considering the coupled fermion–boson system which was used in previous works [25,26]. While the first method is based on unitary transformation which estimates the contribution of whole independent boson system, the other one is the non-equilibrium Green's function to calculate the transport through the nano structure.

2. Method and results

2.1. The electronic and Hubbard model

The pure electronic Hamiltonian of the T-GQD contains the non-interacting and the Hubbard term

$$H_{T-GQD}=\sum_{i,\sigma}\varepsilon_i C^{\dagger}_{i,\sigma}C_{i,\sigma}+\sum_{<i,j>,\sigma}t_{ij}[C^{\dagger}_{i,\sigma}C_{j,\sigma}+C^{\dagger}_{j,\sigma}C_{i,\sigma}]+U\sum_{i,\sigma}C^{\dagger}_{i,\sigma}C_{i,\sigma}C^{\dagger}_{i,\sigma'}C_{i,\sigma'}, \tag{1}$$

where ε_i is the on-site energy of carbon atoms and $t_{ij}$is the hopping between nearest neighbor atoms. $C^{\dagger}_{i,\sigma}(C_{i,\sigma})$is the electron creation (annihilation) operator for an electron with spin σat site i. The last term in the Eq. (1) describes the interaction between electrons with opposite spin on the same site. The strength of interaction, U will be considered as a parameter in our calculations. The Hubbard Hamiltonian can be discussed in the mean-field sense [20,22–24] and Configuration–Interaction (CI) [19,21,22] methods. Here we have used the mean field approach which has been discussed in literatures. In this work, our main concern is to focus the effect of electron–photon interaction term on the transport properties of nano device.

2.2. Electron–photon interaction

In the next step, we consider a T-GQD between two semi-infinite leads as left and right electrodes in the presence of electron–photon interaction as shown in Fig. 1.a for a dot with N atoms in the zigzag edge.

The matrix form of the total Hamiltonian of the above described system in the presence of electron photon interaction can be written as,

$$H=\begin{bmatrix} H_L & H_{L,GQD} & 0 \\ H^{\dagger}_{L,GQD} & H_{T,GQD}+H_{e-ph} & H^{\dagger}_{R,GQD} \\ 0 & H_{R,GQD} & H_R \end{bmatrix} \tag{2}$$

where $H_{L/R}$ and $H_{L/R,GQD}$ are Hamiltonians of left/Right electrodes and the coupling between electrodes and T-GQD, respectively. Here, the contribution of electrodes in the Hamiltonian of system is modeled by specifying the self-energy of left and right electrodes $\Sigma_{L/R}$. For the sake of simplicity, the self-energy of electrodes are written in the simple wide-band approximation. In this approximation the imaginary part of self-energy is considered a constant number and the real-part is ignored. H_{e-ph} describes the electron–photon interaction in the central region which is zero in the case of dark condition.

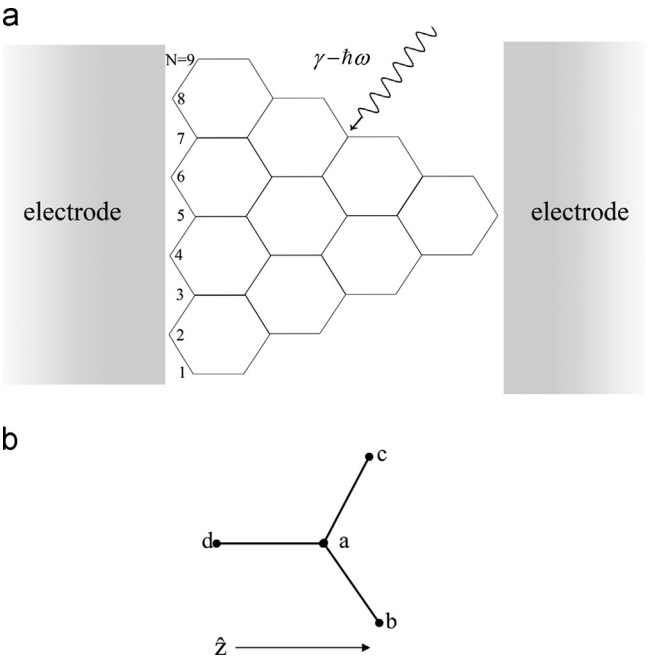

Fig. 1. (a) The schematic structure of T-GQD between two semi-infinite electrodes in the presence of light illumination. (b) Different bonds between carbon atoms.

The Hamiltonian of the electron–photon interaction is written as

$$H^{e-ph}=\frac{e}{m}\mathbf{A}.\hat{\mathbf{p}} \tag{3}$$

A is the vector potential of the electromagnetic wave and **p** is the momentum operator. The vector potential in term of the bosonic creation (annihilation) operator $b^{\dagger}$ (b) is written as

$$\mathbf{A}(x,t)=A_0(x)(be^{-i\omega t}+b^{\dagger}e^{+i\omega t}), \tag{4}$$

In a semi-classical approach for N^{ph} photons in volume V with dielectric coefficient ε_0, $A_0=\hat{\varepsilon}(N^{ph}\hbar/2\varepsilon_0 V\omega)^{1/2}$. The $\hat{\varepsilon}$ is a unit vector which shows the polarization of electric field. If the polarization of electric filed assumed in the z direction which is perpendicular to the transport direction [27].

$$H^{e-ph}=ie\sqrt{\frac{N^{ph}}{2\varepsilon_0 V\hbar\omega}}\sum_{m,n}(z_n-z_m)\langle m|H_0|n\rangle(be^{-i\omega t}+b^{\dagger}e^{+i\omega t})C^{\dagger}_m C_n$$
$$=\sum_{m,n}M_{m,n}(be^{-i\omega t}+b^{\dagger}e^{+i\omega t})C^{\dagger}_m C_n, \tag{5}$$

$M_{m,n}$ are the matrix elements of the interaction. In the case of a hexagonal structure, the matrix elements of interaction are

$$M_{a,x}=\begin{cases} M_0=ie\sqrt{\frac{N^{ph}}{2\varepsilon_0 V\hbar\omega}}\sin(\frac{\pi}{3})a_{C-C}t_{C-C} & x=b \\ -M_0 & x=c \\ 0 & x=d,\ else, \end{cases} \tag{6}$$

where a, b, c and d are atomic positions according to Fig. 1.b. M_0 contains the energy and the number of photon which corresponds to the intensity of incident light. In the presence of electron–photon interaction, the total Hamiltonian of the isolated structure from electrodes is $H=H_{T-GQD}+H^{e-ph}$. The electron–photon interaction includes also a term $\sim C^{\dagger}_i C_j$ which permits the particle to change its state by emitting or absorbing a photon. Independent boson models, such terms make Hamiltonian unsolvable, and in most cases their contributions are omitted [28]. Due to the this