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Quantized Conductance in Graphene based Coherent Nano-Structures

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Abstract

Quantum interference by electronic waves very significantly influences the quantum transport and hence the electronic properties in nanomaterials. Graphene, in which the Dirac fermions play an important role in transport, is studied through one such transport parameter e.g. conductance. Graphene quantum dot of two different shapes and sizes are considered for the study. The conductance is seen to oscillate with electron energy. Size of the ballistic leads also affects the size of the oscillations.

Keywords : Graphene, Dirac Fermions, Quantum Dot, Tight Binding Model, Ballistic Conductance.

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1. Introduction

Graphene, an allotrope of carbon with sp^2 interbonding, consists of a two-dimensional sheet of hexagonal arrangement of carbon atoms forming a lattice of honeycomb structure. Due to its high electron mobility, graphene can transfer electrons at much faster speed compared to silicon. Long range ballistic transport with sustained appreciable phase-relaxation path makes graphene based devices coherent. Coherency is the result of elastic nature of all electron-electron and electron impurities collisions. Also, the pristine graphene - a microscopic planes sheet of graphene is extremely strong impermeable film. Due to its twodimensional structure, graphene shows many interesting features in its electrical, optical and mechanical properties. At and near corner points (Dirac points) of the hexagonal Brillouin zone, the electrons behave as mass-less photons [1-3] on account of linear energy dispersion relation,

$$E = \hbar v_f k$$

where E being the electron energy, V_F n the Fermi velocity and k the wave vector.

Conductance plays a key role in transport through nanodevices. Study of transport in graphene devices opens up amazing interests [4]. The intriguing fluctuations of conductance under different physical conditions and at different sizes and shapes have been reported in a number of literatures [5-7].

In this paper, computational study of conductance in graphene nanostructures is made. Remaining part of the paper is organized as follows. Section 2 outlines the E-k dispersion relation in the tight binding framework. Section 3 deals with computation and simulation. Physical interpretations of the simulated results are discussed in Section 4. Conclusion is made in Section 5.

2. Energy Dispersion

The bonding in the lattice structure of graphene is made by sp^2 interacting orbitals giving rise to the σ band while the pz orbitals overlap giving rise to the π band and are held responsible for the electronic and optic properties of the material. Basic features of nanoscale structures are captured by application of tight-binding (TB) modeling where spatially localized basis functions are used.

2.1 Tight-Binding Model

The band structure calculation is made by use of semiempirical tight-binding approach: Out of the four outer orbital valence electrons ($2s^2\ 2p^2$) of a carbon atom in graphene, three electrons form the covalent sigma bonds to bind the adjacent atoms together, while the remaining electron (valence electron) is responsible to manifest the transport and optic property of the material. In the tight binding approach, the electrons are assumed to be tightly bound to a single atom with interaction potentials from a few nearby atoms. These interacting potentials are treated as perturbation to the main Hamiltonian of any arbitrary electron located in the field of its parent nucleus. This is represented as

$$H \quad -\frac{\hbar^2}{2m^*}\nabla^2 \quad \sum_{m\ 1}^{N} \mathrm{V}(\vec{r}-\overrightarrow{R_m}) \qquad (1)$$

where V is the potential energy of the electron at position $\vec{r}$ due to all N number of positive ions located at positions $\vec{R}_m s$. m^* the effective mass of electron. In the tight-binding formalism, the pz orbitals and the nearest neighbor hopping are assumed. All the atomic orbital wave functions contributed from all the atoms superimpose to generate the wave function of any electron in the crystal system.

The time independent nth state eigen value Schrodinger equation is

$$E_n\ \vec{k} \quad _n\ \vec{k},\vec{r} \quad \hat{H}\ _n\ \vec{k},\vec{r} \qquad (2)$$

$\hat{H}$= Hamiltonian operator

$E_n(\vec{k})$=nth state energy eigen value

$_n\ \vec{k},\vec{r}$ =nth eigen wave function

$\vec{k},\vec{r}$ being the wave vector and position respectively. The electron energy is calculated from

$$E_n\ \vec{k} \quad \frac{\langle \psi_n\ \vec{k},\vec{r}\ |\hat{H}|\psi_n\ \vec{k},\vec{r}\ \rangle}{\langle \psi_n\ \vec{k},\vec{r}\ |\psi_n\ \vec{k},\vec{r}\ \rangle} \qquad (3)$$

Expanding the electron wave functions $_n\ \vec{k},\vec{r}$ in the crystal in terms of known functions, called Bloch orbital basis functions $\phi\ \vec{r}$, we write

$$\psi_n\ \vec{k},\vec{r} \quad \sum_{m\ 1}^{N} a_m\ \vec{k}\ \phi_m\ \vec{r}-\overrightarrow{R_m} \qquad (4)$$

where ϕ is the atomic orbital, m is the lattice site and nis equal to the number of states in the basis.

The basis functions $\phi_m s$ s are all bloch orbital functions due to translational symmetry, and the coefficients $a_m s$ are simply the phase factors, i.e.

$$a_m\ \vec{k} = e^{i\vec{k}\cdot\vec{r}} = e^{ikma}$$

Substituting equation (4) in equation (3) andmultiplying both sides of equation (3) by ϕ_n^* we get after integration the matrices

$$E_n\ \vec{k} \sum_m s_{nm}\ \vec{k}\ a_m\ \vec{k} \quad \sum_m H_{nm}\ \vec{k}\ a_m\ \vec{k} \qquad (5a)$$

where 'a' is the column vector of m elements, H_{nm} is the Hamiltonian matrix element of the atomic orbitals ϕ_n and ϕ_m, s_{nm} is the overlap matrix element of orbitals ϕ_n and ϕ_m.

Obviously, size of the matrices [H] and [S] are determined by the number (n = m) of basis functions.

The equation (4a) may be rewritten in the matrix form of

$$E_n\ \vec{k} \quad S \quad a_m \quad H \quad a_m \qquad (5b)$$

The energies are given by solutions of the secular equation

$$\det\left[E_n\ \vec{k}\ S-H\right] \quad 0 \qquad (6)$$

The honeycomb graphene is analyzed as a bipartite lattice with two-atom unit cell as a Bravais lattice. Size of the matrices are determined by total number of basis function in one unit Bravais cell [8]. Thus, the size of the transfer integral matrix [H] and that of the overlap integral matrix [S] may be represented by 2×2 matrices:

$$H \quad \begin{matrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{matrix} , \qquad S \quad \begin{matrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{matrix}$$

where, $H_{nm} \int \phi_n^* \hat{H} \phi_m$ and $S_{nm} \int \phi_n^* \phi_m$

The n,n and n,m elements are the on-si off-diagonal nearest- neighbor (nn) ho respectively. The [S] matrix is an identity matrix.

In the tight-binding approach, the bas the atomic wave functions of the in Thus in an unit cell of graphene containing we assume two basis functions in total.

2.2 Ballistic conductance in Graphene:

A graphene nano-structure is electrostat to two large contacts by two coherent leads (Fig. 1):

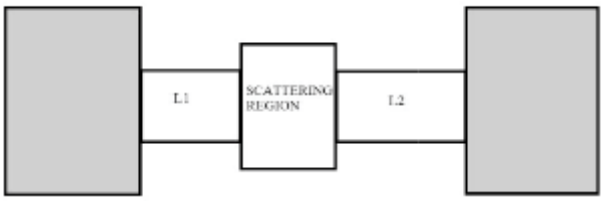


Figure1: Coherent transport of multim through a system of scattering region with two leads L1 and L2.

Considering the contacts to be reflectionless, one gets the conducatance between two contacts as,

$$G \quad \frac{2e^2}{h} \bar{T} \ (E) \qquad (7a)$$

where e and h being electron charge and Planck's Constant respectively and T (E) is the total transmission given by,

$$\bar{T} \ E \quad \sum_{m \ n} T_{nm}$$

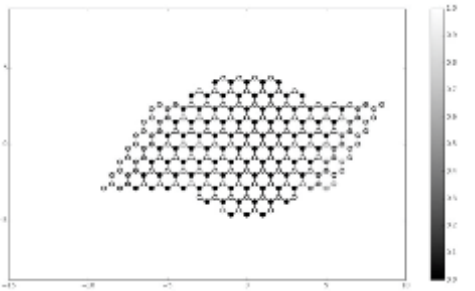
where T_{nm} is the transmission probability of an electron in a mode m at lead 1 emerging out of the scatterer in a different mode n progressing through lead 2. The sum goes over all the input and the output modes propagating through all the leads. Thus the conductance may be obtained from transmission. Also,

$T_{nm} \quad |s_{nm}|^2$, s_{nm} being the (n,m) element of the scattering matrix corresponding to the transmission probability matrix element (n,m) of T_{nm} Thus,

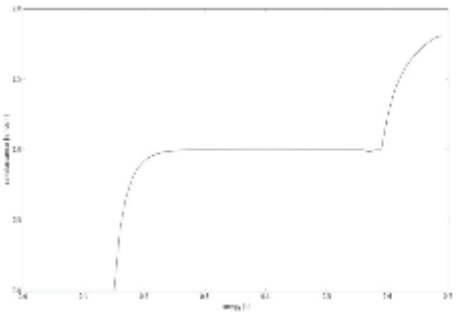
$$G \quad \frac{2e^2}{h} \sum_m \sum_n |s_{nm}|^2 \qquad (7b)$$

3. Computation and Simulation

For numerical computation and simulation we have considered a system of quantum dot (QD) with two semi-infinite leads on hexagonal honeycomb lattice of graphene. Two different shapes viz. circular and square of graphene nano-dot are taken as examples. The conductance is computed using equations (7) and simulated by Python programming. Lattice constant and nearest-neighbor hopping energy are taken as 2.465 nm and 2.7 eV respectively as cited in literatures elsewhere. The simulated plot of circular quantum dot of graphene with two identical leads is shown in Fig.2.(a) and that of the conductance is shown in Fig.2.(b).



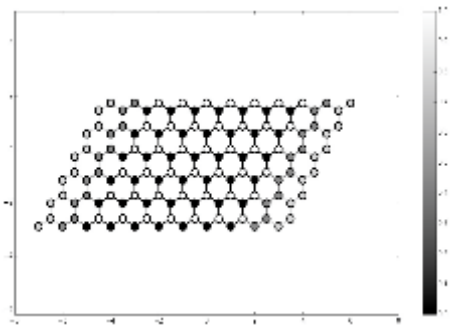
(a)



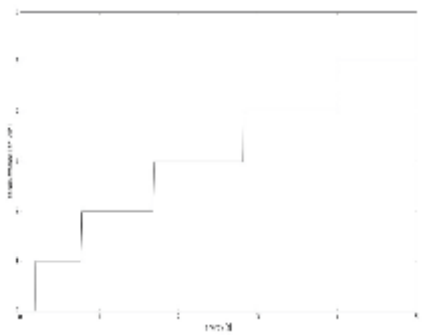
(b)

Figure 2: Plot of (a) circular quantum dot of radius =5 nm and lead width = 6nm (b) conductance vs. energy of dot structure (a)

Similar simulations are also repeateated for square shaped 5 x 5 nm quantum dot as shown in Fig.3.(a) and Fig.3.(b) respectively.

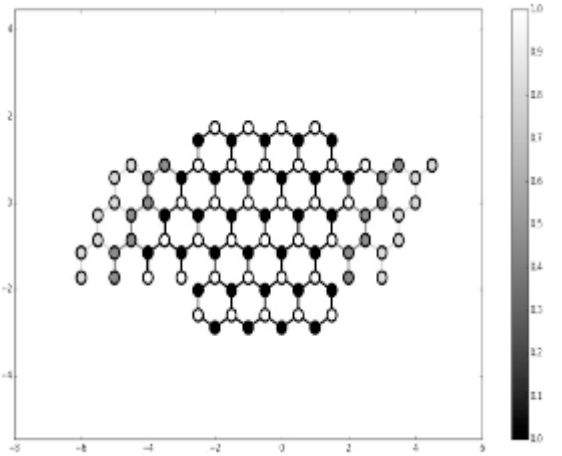


(a)

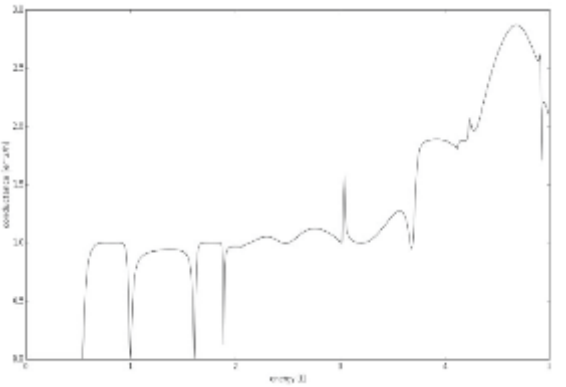


(b)

Figure 3: Plot of (a) square shaped quantutum dot. 5 x 5 nm and lead width 5nm (b) conductance vs energy of dot structure (a)



(a)



(b)

Figure 4: Plot of (a) square shaped quare shaped quantum dot. 5 x 5 nm and lead width 3.33 nm (b) conductance vs. energy of dot structure (a)

4. Results and Discussion

Unlike the Ohmic transport, the transport through the leads is ballistic and coherent. This is because of the fact that electron beam passing through a real conductor may be conceptualized to incoherent beam splitting by way of scattering centres in defects or otherwise. Fluctuating scattering centres help in the process of phase relaxation. These phase relaxation lengths are short enough that the interference effect is neglected. This makes the transport coherent and ballistic. From Figs.(2b)

and (3b) we note the discrete steps heights of $2\frac{e^2}{h}$ in the conductance profile. This is quite expected from the equations (6) where the total transmission probability *T (E)* depends upon number of modes formed in the lead. This, in turn, depends upon the width of the lead. Lead width equaling or comparable to the dot size makes the transport two dimensional (2D) in character. This is reflected by the step profiles in Figs.(2b) and (3b). Gradual decreasing lead width compared to the dot-size deviates transport from that in 2D. Figure(4a) shows the structure of a square QD of same size but of relatively small lead width. This is manifested as complex oscillations of the conductance as depicted in Fig.(4b).

5. Conclusions

Conductance in graphene nano-dot exhibits interesting variations under different conditions of its shape and size. This opens up graphene nano-structures' unique use in device performance of specific applications. Second and higher order models are expected to yield better results.

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