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Electronic transport in rhombus and bowtie graphene nanoflakes

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ABSTRACT

The electrical conductance of two kinds of graphene nanoflakes (GNFs) is studied numerically, using non-equilibrium Green's function. We perform the calculations on bowtie and rhombus GNFs within the nearest neighbor tight binding model. Our findings reveal the sensitivity of conductance on the orientation of zigzag edges. The results show that the conductance of the bowtie and rhombus GNFs could be tuned via enlarging the system size. Moreover, we obtain different results for conductance of the mentioned GNFs and rectangle zigzag GNF with the same size.

1. Introduction

Since the experimental realization of graphene [1], enormous scientific and industrial interest arrived due to its promising electrical, optical, thermal, and mechanical properties [2,3]. The gapless nature of graphene [4] limits its applications in the fabrication of novel electronic devices. Band gap can be induced and tuned by several methods such as doping [5], gating [6] and by applying electric field [7,8]. One common strategy is to create graphene nanoribbons (GNRs) by cutting a graphene sheet along a certain direction [9,10]. Due to the existence of a significant number of atoms at the edges of GNRs, which play an important role in modifying the electronic properties, band gap can be opened up tunably in GNRs depending on their width and type [11,12]. However, cutting graphene sheets into GNRs leads to electron mobility degradation, which limits its performance in devices [13]. GNRs can be classified in two different groups according to their peripheral shape, which are named armchair and zigzag graphene nanoribbons (ZGNRs).

In recent years graphene nanoflakes (GNFs), arbitrarily shaped graphene fragments that are finite in both dimensions, have emerged as new materials for improving electronic, spintronic, optical and sensing devices [14]. Mono-layer and multi-layer flakes can be generated by different techniques [15]. The increasing interest in these materials is connected with the progress in the fabrication of low-cost GNF samples, since they exist widely in nature [16], with a reasonably high degree of control [17,18]. The aspect ratios of GNFs (length divided by width) typically is of the order of unity [19], but in the case of GNRs the aspect ratio in the lateral plane takes value greater than about 10 [20,21].

The potential applications of GNFs arise from their quantum confinement and variation of the edges. This is due to the fact that they can be cut into a much larger variety of different shapes [22,23]. Shrinking system size to quantum levels, comparable to de Broglie wavelength of charge carriers, makes the energy levels discrete and this tunes up the band gap [24]. The quantum size effect in nanostructures generates novel properties that can hardly be seen in the bulk, such as the conduction-insulator and nonmagnetic-magnetic transition of noble nanoscale materials. The extraordinary electronic and optical properties of such quantum dots attract interest for their applications in sensors, catalysis, supercapacitors, bioimaging, luminescence, and spintronic devices [25–28]. In addition to the features inherited from graphene and GNRs, corner states which are formed where two edges meet each other, are unique to GNFs [13]. Furthermore, early studies suggest that small GNFs have discrete electronic structure, which changes to a continuous band structure as their dimension grows [29]. Therefore, the basic change in the nature of the electronic level leads to the potential applications of GNFs from molecular to semi-infinite 2D electronic devices [13]. Several research teams show that GNF's electronic and magnetic properties depend significantly on size, shape, edge geometry, passivation, stacking, twisting, and terminal functional groups [30–36].

The electronic properties of several highly symmetrical GNF shapes such as triangular, hexagonal and other polygonal shapes have been studied [37–40]. Exploring different shapes of GNFs to

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take over the gapless nature of graphene has triggered numerous studies. In this work, we investigate rhombus and bowtie shape of GNFs, which are made from triangular shape using non-equilibrium Green's function theory. These GNFs are obtained by removing different number of hexagons from a rectangle zigzag GNF (RZGNF) monolayer. We also check the dependence of transport properties of both considered nanoflakes on shape and size of the system, and compare them with a same width and length of RZGNF. Totally, we try to tune the band gap of the mentioned GNFs by changing their different features.

We find that, these two types of GNFs with zigzag boundaries have semiconducting behavior in contrast to the ZGNR which is always metallic. The semiconducting behavior of the studied GNFs is expected, since the non-straight zigzag edges play a complex role in transport mechanism. Quantum confinement and variations of the edges in rhombus and bowtie GNFs give rise to rich electronic properties with some exotic phenomena. An interesting point to keep in mind is that, transmission of RZGNF shrinks by decreasing its aspect ratio, as predicted by quantum confinement theory.

The remaining sections are organized as follows. In Section 2 we will briefly describe the NEGF method used for calculation of conductance in GNFs. Section 3 is dedicated to illustrate and discuss the results from our calculations. Finally, we conclude and give a summary of our main findings in Section 4.

2. Non-equilibrium Green's function method

From a mathematical viewpoint, Green's function is an integral kernel to solve differential equations with initial or boundary conditions [41]. Non-equilibrium Green's function (NEGF) method is one of the best and powerful theoretical methods to study electrical transport in nanostructures [42]. The predicted values by NEGF calculations are in agreement with what was experimentally observed [43].

In order to mimic a real experiment, we put our nano-device between two semi-infinite electrodes as charge source and drain, to calculate its electrical conductance. A schematic view of the system is depicted in Fig. 1. Here, the systems under consideration are rhombus and bowtie GNFs with different width and length, which we have cut them from rectangle ZGNFs into these shapes by removing carbon atoms. We choose two semi-infinite ZGNRs as left and right leads connected to central device.

We start from Schrödinger equation for central device:

$$(E - H)\Psi = f(x), \tag{1}$$

where E denotes charge carriers energy and Ψ is electronic wave function. In this case, the wave function can be interpreted as system's response to an excitation $f(x)$. Hamiltonian H represents isolated Hamiltonian of device H_{device}, modified by boundary conditions, which are included in self energy function: $H = H_{device} + \Sigma$. Self energy contains the interaction of central device with left and right contacts: $\Sigma = \Sigma_L + \Sigma_R$. $\boldsymbol{H}_{device}$ matrix for a device containing N atoms, can be written by using a nearest neighbor tight-binding model with P_z orbital basis set,

$$\boldsymbol{H}_{device} = \sum_{i=1}^{N}(|\, i > H_{i,i} < i\,|) + \sum_{<i,j>}(|\, i > H_{i,j} < j\,|), \tag{2}$$

where $H_{i,i}$ is the on-site energy, and $H_{i,j}$ is the hopping energy between nearest neighbor lattice points i and j. $|i>$ shows the state vector of i-th site in the device, and $\sum_{<i,j>}$ refers to a sum over the nearest-neighbor sites. In zero-bias voltages, the value of on-site energy and hopping energy are chosen to be zero and 2.7 eV, respectively.

The corresponding retarded Green's matrix, $\boldsymbol{G}^r$, of the central device can be obtained by solving the equation

$$[(E + i\eta)\boldsymbol{I} - \boldsymbol{H}]\,\boldsymbol{G}^r = \boldsymbol{I}. \tag{3}$$

The energy, E, is measured with respect to the Fermi energy, E_F, and $i\eta$ is an arbitrary infinitesimal imaginary number added to energy for ensuring convergence of the above equation. $\boldsymbol{I}$ and $\boldsymbol{H}$ denote identity matrix and Hamiltonian of central device, respectively. Thus $\boldsymbol{G}^r$ has a well-known form [44,45]:

$$\boldsymbol{G}^r(E) = \left[(E + i\eta)\boldsymbol{I} - \boldsymbol{H}_{device} - \boldsymbol{\Sigma}_L^r - \boldsymbol{\Sigma}_R^r\right]^{-1} \tag{4}$$

The coupling matrix (self-energy) between left/right lead and central device is defined as

$$\boldsymbol{\Sigma}_{L/R}^r = \boldsymbol{\tau}_{L/R}^{\dagger}\boldsymbol{g}_{L/R}\boldsymbol{\tau}_{L/R} \tag{5}$$

where, $\boldsymbol{\tau}_{L/R}$ is referred to as the coupling matrix, which shows the hopping of electron from the left/right electrode to the device. $\boldsymbol{g}_{L/R}$ is the surface Green's function of left/right lead, which is calculated by using Dyson's equation with an iterative procedure [46,47]:

$$\boldsymbol{g}_{L/R}(E) = \left[(E + i\eta)\boldsymbol{I} - \boldsymbol{H}_0 - \boldsymbol{H}_1\boldsymbol{g}_{L/R}(E)\boldsymbol{H}_1^{\dagger}\right]^{-1}, \tag{6}$$

where $\boldsymbol{H}_0$ and $\boldsymbol{H}_1$ are the Hamiltonian of one isolated layer of the lead and the hopping between neighboring layers, respectively. It should be noted that the surface Green's function in the first step of iteration process is calculated by $\boldsymbol{g}_{L/R}(E) = [(E + i\eta)\boldsymbol{I} - \boldsymbol{H}_0]^{-1}$.

In NEGF theory, the transmission probability of carriers through the device at energy E, $T(E)$, can be written as [48]:

$$T(E) = Tr\left[\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^r(E)\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^a(E)\right], \tag{7}$$

where $Tr(\boldsymbol{X})$ gives trace of matrix $\boldsymbol{X}$. $\boldsymbol{G}^a = [\boldsymbol{G}^r]^{\dagger}$ is advanced Green's function of the center device area, and $\boldsymbol{\Gamma}_L$ ($\boldsymbol{\Gamma}_R$) is the contact-broadening function describing the coupling between central device and left (right) lead. The coupling matrix, which is the energy level broadening matrix due to the source (drain) contacts, can be obtained from the self energy terms via the below formula:

$$\boldsymbol{\Gamma}_{L/R}(E) = i\left[\boldsymbol{\Sigma}_{L/R}^r(E) - \boldsymbol{\Sigma}_{L/R}^a(E)\right]. \tag{8}$$

Once Hamiltonian and self energy terms are known, all quantities of interest can be calculated from Eqs. (4) and (7). Transmission coefficient is related to electrical conductance: $T = G/G_0$, where $G_0 = 2e^2/h$ is referred to as conductance quantum.

Fig. 1. Schematic view of the system consisting of three parts: left lead, central device, and right lead.