Kordbacheh et al. Journal of Theoretical and Applied Physics 2013, 7:54
http://www.jtaphys.com/content/7/1/54

Journal of Theoretical and Applied Physics
a SpringerOpen Journal

RESEARCH Open Access

Abnormal electronic transport in disordered four-terminal graphene nanodevice

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Abstract

In this paper, a numerical study of quantum transport in a disordered four-terminal graphene nanodevice is investigated based on the Landauer approach. The effects of impurity on transmission coefficient of the electron injected into the system are studied using tight-binding model. In this manner, we emphasize that when the disorder density is sufficiently large, the transmission coefficients and the current reduce due to multiscattering phenomenon. We have found that the perfectly conducting channel develops in four-terminal device in its zigzag edge if the range of impurity gets exponentially wider. The theoretical results obtained can be a base for the development in designing graphene nanodevice.

Keywords: Quantum transport; Graphene nanodevice; Transmission coefficient

Introduction

The problem of impurity in systems with Dirac fermions has been studied extensively in the last few years [1,2]. Understanding the role of the defects in the transport properties of graphene is central to realize future electronics based on carbon. It has been shown recently that charge carriers in graphene are massless Dirac fermions with effective 'velocity of light,' and it is well known that disorder is ubiquitous in graphene and its effect on the electronic structure has been studied [3-5]. The electron transport in one-dimensional (1D) carbon systems displays unusual properties, in apparent opposition with the common belief that 1D systems are generally subjected to Anderson localization [6,7].

Unlike carbon nanotubes, graphene ribbons have edges that are vulnerable to impurity that could limit the localization length, and hence, the length over which ballistic transport could occur.

It was shown that carbon nanotubes with long-ranged impurities possess a perfectly conducting channel (PCC) [8,9]. Based on the critical role that two-dimensional multiterminal devices have played in semiconductor nanotechnology, multiterminal graphene devices should also play an important role in any graphene-based electronic circuits [10]. In addition to the practical importance of these multiterminal graphene devices, these systems make a useful framework to study the effect of lattice defects on the electron transport in the device. In this paper, we perform calculation to investigate the effect of the impurity potential range and its density on the conductance of four-terminal graphene nanodevice and we have found that the PCC develops in the four-terminal device.

Theoretical model

We consider the system as a central conductor region (C), connected to four leads L, R, B, and T (see Figure 1). The leads are formed by semi-infinite perfect ribbons, simulating four ideal leads. The conductor region consists of N_c number of atoms.

The tight-binding Hamiltonian of the system can be written as [11,12]

$$H = \sum_i \varepsilon_i a_i^+ a_i + t \sum_{i,j} e^{i\phi_{ij}} a_i^+ a_j + \sum_i V a_i^+ a_i, \qquad (1)$$

where a_i and a_i^+ are the annihilator and creator operator of the electron; t is the hopping integral between the nearest neighbors. In the absence of impurity, ε_i is taken to be zero and t = 2.7 eV. In the presence of disorder, N_i impurities are randomly distributed among N_c sites. The

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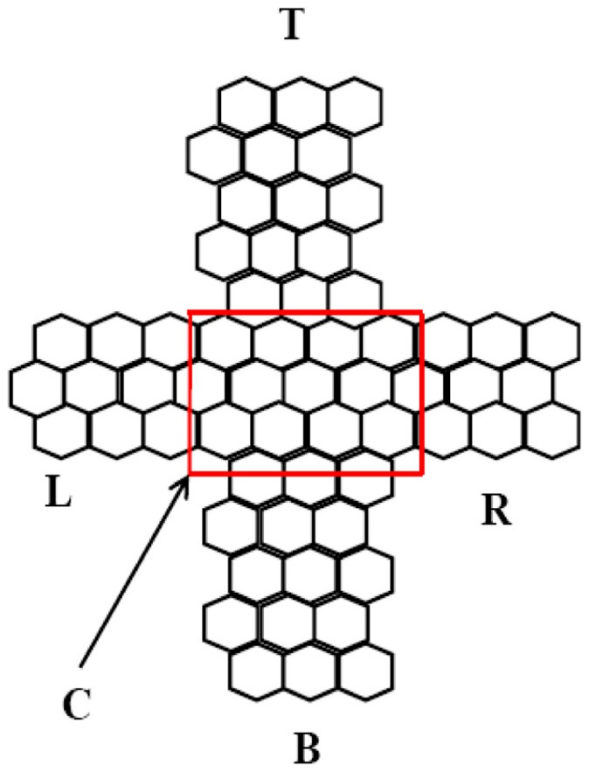

Figure 1 Lattice configuration of four-terminal graphene device. Central region (boxed) is the conductor region, C, which is attached to four leads L, T, B, and R.

potential energy of the ith site at position r_i is induced by these impurities as [11,12]:

$$\varepsilon_i(r_i) = \sum_{n=1}^{N_i} V_n \exp\left(-|r_i - r_n|^2/\left(2d^2\right)\right), \quad (2)$$

where r_n is the position of the nth impurity, d represents the spatial range of the impurity potential, and the potential strength V_n of the impurities is randomly distributed in the range ($W/2$, $W/2$) independently. We emphasize that the potential that we consider, being static, does not actually break the time reversal symmetry in graphene.

In what follows, we show how to calculate the transmission of the system. In the absence of thermal effects and the charging terms, the transmission coefficient for electrons from the left lead to the right lead with energy E is related to Green's functions using Caroli's formula which provides high numerical accuracy and efficiency:

$$T = Tr\left(\Gamma_m G_c^r \Gamma_n G_c^a\right), \quad (3)$$

where $G_c^{r,a}$ are the retarded and advanced Green's functions of the conductor, and $\Gamma_{m,n}$ are coupling matrices from the conductor to the leads. The systems have four leads, resulting in a conductor Green function of form [12,13]

$$G_c^r = \left[(E + i\eta)I - Hc - \sum\nolimits_{\mathrm{L}}^r - \sum\nolimits_{\mathrm{R}}^r - \sum\nolimits_{\mathrm{T}}^r - \sum\nolimits_{\mathrm{B}}^r\right]^{-1}, \quad (4)$$

where I is the identity matrix, $\sum_n$ denotes self-energy due to the coupling between the conductor and lead n; $i\eta$ is a small imaginary term added to make the Green's function (G) non-Hermitian. When there are more than two leads, the matrix algebra in (3) is somewhat more complex as described in [14]. The coupling matrices are expressed as:

$$\Gamma_n = i\left[\sum\nolimits_n^r - \sum\nolimits_n^a\right]. \quad (5)$$

The function Γ_n is called the broadening function and describes the coupling of the device to the leads, where $\sum_n^r = \left(\sum_n^a\right)^+$. The conductor region consists of N_c atoms (where N_c = 32), making all the matrices $N_c \times N_c$ square matrices.

Integrating the transmission probability over the whole energy range and for the external bias applied to the electrodes, one can derive the tunneling current as the form

$$I(V,T) = 2e/h \int T(V,E)[f(E-\mu_n) - f(E-\mu_m)]dE, \quad (6)$$

where T (V,E) is the transmission probability per energy E, f (E) is Fermi-Dirac distribution, V is the bias voltage applied to the system, and $\mu_m(\mu_n)$ is the chemical potential at $n(m)$ lead ($\mu_m = \mu_n + \mathrm{eV}$). The conductance $G(E)$ of the four-terminal graphene can be calculated using the Landauer formula [12,13]:

$$G = \left(2e^2/h\right)T \quad (7)$$

where h is the Planck's constant and e is the electron charge.

Results and discussion

Firstly, we investigate the effect of the potential range d and density ni ($ni = N_i/N_c$) of the impurities with fixed $W = 0.5\,t$. In Figure 2, we plot the transmission coefficients of electrons injected to the four-terminal graphene device as a function of energy with different potential range d at fixed impurity density ni = 30 %. electrons are injected through the zigzag ribbon from L to R. A direct conclusion from this figure is that in most regions of E, short-range (d = 0, a) impurities (SRI) can lead to a considerable decrease of conductivity, but long-range (d = 3a) impurities (LRI) will decrease the transmission much further, in the case of the same impurity density.

The fine peaks in pure case, known as Van Hov singularities (VHSs) [15], correspond to the extreme points in the energy bands (the critical point found in phase diagrams is a completely separated phenomenon); however, the peaks in the transmission of disordered case correspond to the impurity states.

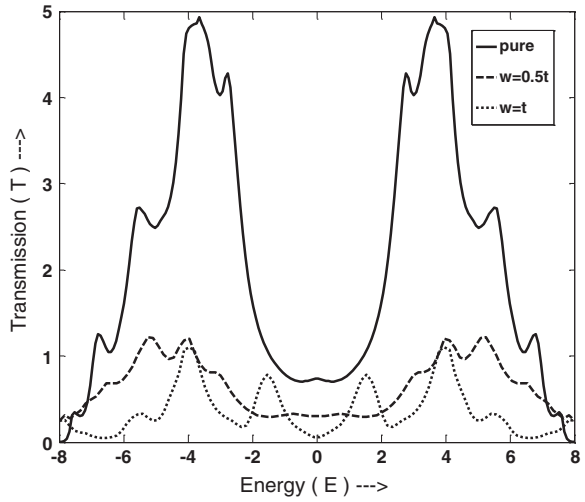

Figure 2 Transmission coefficients of electrons with different impurity potential at fixed impurity density. The transmission coefficients of electrons injected to the four-terminal graphene nanodevice as a function of energy with different impurity potential (W) at fixed impurity density $ni = 30\%$ with impurity range $d = a$. The curve for a device without any impurities is also plotted as a reference.

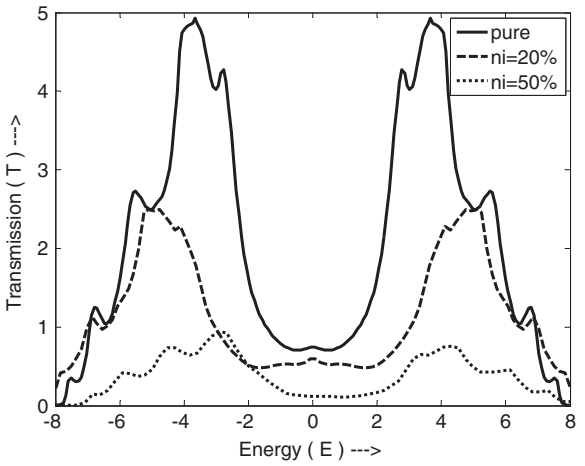

Figure 3 Transmission coefficients as a function of energy with different impurity density at fixed impurity range. The transmission coefficients as a function of energy with different impurity density at fixed impurity range $d = a$ and $W = 0.5\,t$.

The impurity states are quasilocalized states caused by the disorder [16]. The injected electron will be reflected when its energy is equal to the energy level of the quasilocalized states; indeed quasilocalized states in disordered graphene near Dirac points have been observed experimentally and numerically [17].

It should be noted that the SRIs do not destroy the shape of VHSs, while LRIs tend to reduce the conductance and obscure the shape of VHSs. For both monolayer and bilayer graphenes, STM experiments have reported that atomic-size impurities give rise to short-wavelength modulations of the LDOS, associated with intervalley scattering [18].

The electron waves are localized around the impurity site. Thus, the conductance reduction is caused by virtual bound states at the impurity. Localization arises from enhanced intervalley scattering due to the deviation from Dirac dispersion in the strong impurity regime; this intervalley scattering is a result of non-Dirac behavior of the honeycomb lattice in the high-energy region and cannot be avoided by simply increasing the potential range. Besides, it has been realized experimentally by RV Gorbachev et al. that unlike conventional 2D systems, weak localization in bilayer graphene is affected by elastic scattering processes such as intervalley scattering [8].

In Figure 3, we plot the transmission as a function of energy with different impurity density at fixed potential range $d = a$ (SRI case) and $W = 0.5\,t$. Disorder causes electron scattering. The quantum scattering theory of free particles in infinite space is a textbook subject, which has been recently scrutinized for massless Dirac fermions in infinite 2D space. Although scattering in graphene can be suppressed because of the symmetries of the Dirac quasiparticles, it is shown that when its source is atomic-scale lattice defects, wave functions of different symmetries can mix [19].

In the case of low-density impurities, the scatterings due to different impurities are independent. But when the density is sufficiently high, the potential field induced by different impurities overlap and multiscattering dominates. This multiscatterings decrease the conductance, which is due to the asymmetric behavior on transmission coefficients.

Figure 4 shows the conductivity as a function of d at zero energy. Our numerical results indicate that transmission is a more complicated function that depends on the nature of the disorder. Clearly, it can be seen that the PCC develops in four-terminal device in zigzag edge

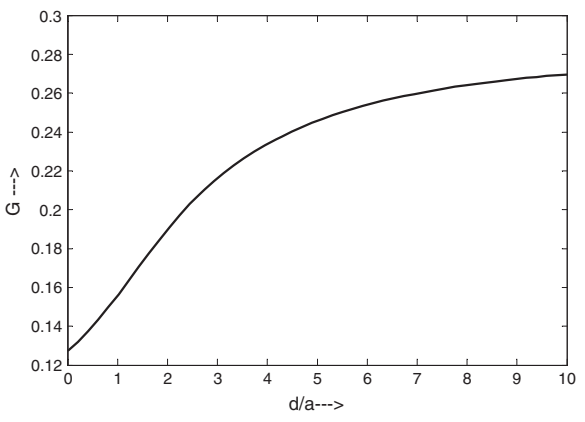

Figure 4 Conductivity as a function of d/a at zero energy.

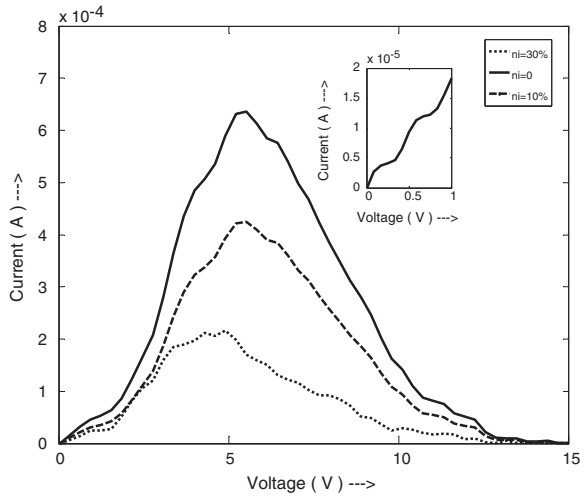

Figure 5 Current–voltage curves of pure four-terminal device with different impurity density. The inset graph shows the current–voltage curve in the vicinity of the Fermi energy.

if the range of impurity gets wide. Since at least one of sub-bands at these energy points gives zero group velocity, it can be considered that the intra-valley scattering becomes stronger and, therefore, behaves in a exponential way in this regime, which is noted as $G \sim \exp(d)$.

In order to investigate the behavior of changes in the current voltage from lead L to lead R, we apply external potential to the system so that lead L lies in the potential of V/2 and lead R lies in the potential of –V/2.

The difference in the transmission coefficients is directly reflected in the current–voltage (*I-V*) characteristics. The current increases linearly due to the finite transmission coefficient near the Fermi energy; these *I-V* characteristics are almost similar to that of the previous work [20]. The overlapping of the states at the right and left leads represents the presence of channel for the injected electrons to be passed. As can be seen in Figure 5, the current increases when we applied voltage to the system. This is due to effective overlapping of two electrodes insofar as the curve's peak shows the enhancement of the overlapping.

The inset graph in Figure 5 shows the current–voltage curve in the vicinity of the Fermi energy; the small oscillations in the curve are due to Van Hov singularity and originated from the 'current quantization' in this mesoscopic system. A direct conclusion from this figure is that low-density impurities can lead to a considerable decrease of current, but high-density impurities will decrease the current much further, in the case of the same range impurities due to multiscattering and Anderson localization; however, curves resume their behavior in most energy regions. By numerical calculation, Liviu P Zarbo and BK Nikoli demonstrated that both short-range and long-range impurities reduce current density in the region of their influence in the single channel transport through the lowest transverse propagating mode generated by the edge states of ZGNR; this reduction in the case of long-range impurities can be compensated by the increase of current density along the zigzag edge, ensuring perfectly conducting channel $G = 2e2/h$ even in the presence of the disorder [8,21].

Conclusions

As a summary, we numerically investigate the transport properties of a four-terminal graphene nanodevice in the presence of impurities with different density and potential range.

We have found that in the presence of impurity, the transmission and current decrease, which means that this impurity can produce the constructive interference. On the other hand, nanographene ribbon with zigzag edges in the four-terminal graphene device possesses perfectly conducting channel if the impurity potentials are long ranged, induced by electronic states which originate from the edge states. These behaviors agree well with the results from a recent experiment.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

The theoretical part of this article has been developed by AAK and AJ. AJ performed all the calculations and the numerical computations. The final manuscript has been read and approved by all the authors.

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AAK is an assistant professor of Physics at Iran University of Science and Technology. AJ is a PhD student of Physics at Islamic Azad University. MS is an assistant professor of Physics at Iran University of Science and Technology.

Acknowledgements

The authors would like to thank the Physics Department of Iran University of Science and Technology for supporting this work.

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Received: 26 February 2013 Accepted: 20 August 2013
Published: 18 October 2013

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doi:10.1186/2251-7235-7-54
Cite this article as: Kordbacheh *et al.*: **Abnormal electronic transport in disordered four-terminal graphene nanodevice.** *Journal of Theoretical and Applied Physics* 2013 **7**:54.