Effect of disorder with long-range correlation on transport in graphene nanoribbon

G P Zhang$^{1,2}$, M Gao$^1$, Y Y Zhang$^3$, N Liu$^4$, Z J Qin$^5$ and M H Shangguan$^1$

$^1$ Department of Physics, Renmin University of China, Beijing 100872, People’s Republic of China
$^2$ Ames Laboratory—US DOE, and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA
$^3$ State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, PO Box 912, Beijing 100083, People’s Republic of China
$^4$ School of Microelectronics and Solid State Electronics, University of Electronic Science and Technology of China, Chengdu 610054, People’s Republic of China
$^5$ School of Physics and Engineering, Zhengzhou University, Zhengzhou 450001, People’s Republic of China

E-mail: zhanggp96@ruc.edu.cn and bugubird_zhang@hotmail.com

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Abstract
Transport in disordered armchair graphene nanoribbons (AGR) with long-range correlation between quantum wire contacts is investigated by a transfer matrix combined with Landauer’s formula. The metal–insulator transition is induced by disorder in neutral AGR. Therein, the conductance is one conductance quantum for the metallic phase and exponentially decays otherwise, when the length of AGR approaches infinity and far longer than its width. Similar to the case of long-range disorder, the conductance of neutral AGR first increases and then decreases while the conductance of doped AGR monotonically decreases, as the disorder strength increases. In the presence of strong disorder, the conductivity depends monotonically and non-monotonically on the aspect ratio for heavily doped and slightly doped AGR, respectively. For edge disordered graphene nanoribbon, the conductance increases with the disorder strength of long-range correlated disordered while no delocalization exists, since the edge disorder induces localization.

(Some figures may appear in colour only in the online journal)

1. Introduction

Graphene, discovered in 2004 [1–4], stimulated intensive research interest in fundamental properties and its potential application in nanoelectronic devices due to its superior properties such as high mobility [3] and heat dissipation [5]. For an infinite pure graphene sheet, the electronic spectrum is linear around the Dirac point and can be described as massless Dirac fermions. Due to its unique electronic structure, many interesting phenomena had been observed such as the half-integer quantum Hall effect [4] and bipolar current [6]. Now it is commonly thought that the most likely application may come from graphene nanoribbons, and the basic types of graphene nanoribbon are armchair-edged and zigzag-edged ones. Defects and impurities are inevitable in graphene-based materials, therefore the effects of defects, impurities and disorder on transport properties are of interest for applications and had been reviewed in [7–10]. As for disorder, it is usually classified as short- or long-range disorder depending on the ratio of the interaction range to the lattice distance [11]. Anderson disorder is a typical short-range disorder and localization is induced by strong disorder. Long-range disorder such as Gaussian-type disorder [12] induces a metal–insulator transition at the Dirac point. After several
years of intensive investigation, it was well known that the scattering between two nonequivalent valleys is absent in the presence of long-range disorder [9]. Interestingly, off-diagonal disorder [13, 14] enhances electronic transport and superconductivity correlation at the Dirac point. Recently, more and more attention was paid to the effect of charged impurities on the transport in graphene-based materials [15, 16] since the observation of electron–hole puddles in graphene [17].

It was commonly believed that Anderson localization [18] in one- and two-dimensional systems is induced by even a weak disorder from scaling theory [19]. It was found that one or several resonant states may occur in a one-dimensional disordered chain with short-range correlation [20–22]. Delocalized states within a continuous energy range exist in one-dimensional systems, when disorder on site energy is long-range-correlated [23, 24], where the energy range exist in one-dimensional systems, when disorder 

\[ \langle \epsilon \rangle \] in one- and two-dimensional systems is induced by off-diagonal disorder [13, 14] enhances electronic transport and superconductivity correlation at the Dirac point.

The geometry of AGR sandwiched by two normal metal contacts is illustrated in figure 1, where semi-infinite quantum wire contacts. The red and blue circles stand for A and B sublattices in graphene ribbon respectively. Two inequivalent lattice vectors \( \vec{a}_1 \) and \( \vec{a}_2 \) are also shown. The shape of GNR is determined by \( L \) and \( M \) carbon atoms in the \( x \) and \( y \) directions, respectively. Correspondingly, the length is \( L_x = \frac{\sqrt{3}L_a}{4} \) and the width is \( L_y = (M - 0.5)a \) with the lattice constant \( a \) being 2.46 Å.

\[ H = t \sum_{ij,j'} C_{ij}^\dagger C_{jj'} + \sum_y (\epsilon_{ij} - \mu) C_{ij}^\dagger C_{ij}, \]

The transport property of GNR is mainly contributed by a \( \pi \) orbital and the tight binding approximation is valid to describe the electronic structure of GNR at the Fermi energy. The Hamiltonian is expressed by

\[ H = t \sum_{ij,j'} C_{ij}^\dagger C_{jj'} + \sum_y (\epsilon_{ij} - \mu) C_{ij}^\dagger C_{ij}, \]

Figure 1. Illustration of armchair graphene nanoribbon (AGR) between two semi-infinite quantum wire contacts. The red and blue circles stand for A and B sublattices in graphene ribbon respectively. Two inequivalent lattice vectors \( \vec{a}_1 \) and \( \vec{a}_2 \) are also shown. The shape of GNR is determined by \( L \) and \( M \) carbon atoms in the \( x \) and \( y \) directions, respectively. Correspondingly, the length is \( L_x = \frac{\sqrt{3}L_a}{4} \) and the width is \( L_y = (M - 0.5)a \) with the lattice constant \( a \) being 2.46 Å.
It is well known that the bandgap of uniform AGR shows a three-family behavior from the tight binding model and first-principles calculation [39], where these two methods predicted that AGR with $N_0 = 3p + 2$ as $p$ being an integer has no bandgap and finite bandgap inversely proportional to the width, respectively. Further it was proved that the bandgap of AGR with $N_0 = 3p + 2$ approaches to zero when the width is wider than 80 Å through a divide-and-conquer approach based on quasi-atomic minimal basis orbits (QUAMBOs) [40]. $N_0$ is $2M$ in AGR as shown in figure 1 and $M = 3p + 1$ stands for metallic AGR. Even for semiconducting AGRs with $M \neq 3p + 1$, the conductance and the localization length always increase with $\alpha$ in the presence of long-range correlated disorder. For the sake of simplicity, metallic uniform AGRs are chosen to investigate the effect of long-range correlated disorder here.

Figure 3 shows the dependence of the conductance on the length of AGR in the presence of several different correlated disorders. As shown in figures 3(a) and (b), the conductance approaches to one conductance quantum at highly correlated weak disorder as the length increases, when $\alpha$ is larger than 2.0 at $\delta = 0.1$. This proves that long-range correlation in disordered onsite energies includes a metallic phase in disordered AGR. On the other hand, the conductance exponentially decays as a function of the length like $G \propto \exp(-aL)$. It implies Anderson localization and $a$ is the inverse of the localization length. $a$ is zero for metallic states and finite for localized states depending on the parameters $\alpha$ and $\delta$. In figure 3(c), the scaling behavior of the conductance shows that there also exists a metal–insulator transition induced by the disorder strength of correlated disorder. From finite size scaling behavior, it is easy to determine the critical $\alpha_{cr}$ in terms of $\delta$ and the critical $\delta_{cr}$ in terms of $\alpha$ from figures 3(a)–(c), respectively. As shown in figure 3(b), $\alpha_{cr}$ is 1.8–1.9 at $\delta = 0.1$. The dependence of conductance on the length of long AGR shows $\alpha_{cr} = 1.86$, which is close to, but a little larger than, the value from the Dirac equation [31]. Moreover, the conductance of the Dirac fermion under disordered potential with long-range correlation scales as $G \propto L^{-\eta}$, in which $\eta$ is a constant and depends on $\alpha$ and $\delta$. The discrepancy comes from the

3. Numerical results and discussion

3.1. The scaling behavior of the conductance at neutral point in the presence of long-range correlated disorder

It is well known that the bandgap of uniform AGR shows a three-family behavior from the tight binding model and first-principles calculation [39], where these two methods
difference of the tight binding model and Dirac equation. However, both the tight binding model and Dirac equation predict a metal–insulator transition induced by the disorder with long-range correlation. Different from neutral AGR, the conductance oscillates around a fixed value and monotonic decay at the energy shift \( \mu \) is 0.2 and 1.0, respectively, when the length increases from 20 to 340, as shown in (d).

### 3.2. Dependence of the conductance on the energy shift in the presence of long-range correlated disorder

Figure 4 shows how the conductance varies with the energy shift at three different strengths of disorder. Here the energy shift in units of the nearest-neighbor hopping amplitude \( t \) is linear to the gate voltage applied to AGR. The size parameter for AGR is \( L = 20, M = 40 \) and \( \alpha = 2.5 \). The conductance of disordered AGR is the average of 500 samples. For comparison, the conductance of uniform AGR is also shown. The slope of conductance at positive energy shift is different from the counterpart at negative energy shift, since the electron–hole symmetry is broken due to an odd-numbered ring at the AGR–QW interface [35]. For weak disorder, e.g. \( \delta = 0.1 \), the conductance curve is slightly different from that of uniform AGR, and asymmetry in electron–hole is still present. As the disorder strength \( \delta \) increases to 0.5, the conductance decreases for most energy shifts while it increases around zero energy shift. The variance of conductance increases with the disorder strength. When \( \delta \) is 1.0, only the conductance near a zero energy shift is highest, which is completely different from those above the curves of the conductance versus the energy shift. Obviously strong localization occurs as the energy shift is far away from zero at \( \delta = 1.0 \).

Figure 5 shows the dependence of the conductance \( G \) at three different energy shifts on the disorder strength \( \delta \). For comparison, \( \alpha = 1.0, 2.0 \) and 2.5 are chosen. As shown in figure 5(a), the conductance of neutral AGR slightly changes with \( \delta \) at \( \alpha = 1.0 \), except that the variance of conductance increases with \( \delta \). The conductance first increases and then decreases as \( \delta \) increases when \( \alpha \) is larger than 2.0. This behavior is similar to that in the presence of long-range disorder [11]. In contrast, the conductance first remains the same at weak disorder and then decays at strong disorder in the presence of short-range disorder such as Anderson disorder. When the energy shift is 0.2, the conductance decreases as \( \delta \) increases for low correlated disorder, and the behavior of the conductance in the presence of highly correlated disorder is similar to that of neutral AGR, as shown in figure 5(b). When the energy shift is 1.0, the conductance decreases as the disorder strength increases for all \( \alpha \) as shown in figure 5(c). This is due to Anderson localization in heavily doped AGR.

It is well known that edge disorder in graphene induces insulating behavior in graphene [41]. Different from complex edge disorder, a simple edge disordered graphene nanoribbon is constructed, in which 5% carbon atoms (i.e. 0.05L and 0.05L) are added randomly to carbon atoms at the top and bottom edges, respectively. Then we analyze the conductance of 100 such random samples in the presence of long-range correlated disorder with \( \alpha = 2.5 \). For each random sample, the conductance is averaged between 500 realizations of long-range correlation disorder, as we did for the case without edge disorder. On the one hand, the conductance increases with the disorder strength \( \delta (\leq 0.5) \), as shown in figure 6. On the other hand, the conductance decreases as the length increases for all \( \delta \), in which no delocalization occurs in the presence of highly long-range correlated disorder. This is contrary to the fact that \( \alpha = 2.0 \) induces delocalization in long-range correlated disordered graphene nanoribbons without edge disorder. The higher per cent edge disorder results in lower conductance, while the dependence of conductance on \( \delta \) is similar. It indicates that no delocalization occurs in edge disordered graphene nanoribbons even when the disorder is correlated, since localization is induced by edge disorder.
Figure 6. Dependence of the conductance on the disorder strength \( \delta \) as the length \( L \) varies from 20 to 60. Full and hollow symbols represent 5\% and 10\% edge disorder. \( \alpha = 2.5 \) and the width of the sample is \( M = 4 \).

3.3. Dependence of the conductivity on the energy shift and on the aspect ratio in the presence of long-range correlated disorder

It is well known that the conductivity of uniform and neutral armchair graphene nanoribbons approaches \( \frac{4e^2}{h} \) as the aspect ratio \( M/L \) is far larger than 1 [42, 43]. The conductivity is defined as \( \sigma = \frac{G L_x}{L_y} \). Figure 7 shows the dependence of the conductivity on the energy shift in the presence of correlated disorder with \( \alpha = 2.5 \) and \( \delta = 1.0 \). Under such parameters as studied in section 3.1, all electronic states are localized at the thermodynamic limit and the conductance decreases as the length increases as shown in the inset of figure 7. Therefore the conductivity approaches to zero as the aspect ratio approaches to zero. However, for moderate aspect ratio, the conductivity increases at \( |\mu| \leq 0.75 \) and decreases otherwise as the length increases from 20 to 100, as shown in figure 7. The transition of conductivity in terms of the length indicates that the conductance scales as \( L^{-\beta} \) with \( \beta \) varying from less than 1 to larger than 1, because the localization length modulated by the energy shift is longer than and shorter than the length of the system \( L \), respectively. We further find that this kind of transition of conductivity occurs in a series of AGRs with different widths.

Figure 8 shows the dependence of the conductivity on the aspect ratio in the presence of disorder with long-range correlation with \( \alpha = 2.5 \) and \( \delta = 1.0 \). Interestingly, there are two different behaviors for conductivity in terms of the aspect ratio. Therein, the conductivity near zero energy shift (\( \mu = 0 \) and 0.2) first increases and then decreases while the counterpart at \( \mu = 1.0 \) monotonically decreases, as the aspect ratio approaches to zero. For comparison, the corresponding behavior of the conductivity for uniform AGR with \( M = 40 \) is also shown. Since the conductance remains finite and constant for metallic AGR, the conductivity scales as \( O(L/L) \) as \( M/L \) approaches to zero for all three different gate voltages. The conductivity corresponding to one quantized conductance is shown by the dotted black line. It is easy to find that the asymptotical conductivity of disordered AGR with long-range correlation is different from metallic uniform AGR, since localization occurs at the thermodynamic limit. On the other hand, the conductivity of disordered AGR at \( \mu = 1.0 \) decreases slower than that of neutral AGR with \( M = 39 \), which is semiconducting without impurity or disorder, while their asymptotical behavior of the conductivity should be the same because of localization. Compared with pure AGR, the conductivity of disordered AGR with long-range correlation depends smoothly on the aspect ratio in general.

4. Summary

Transport in disordered armchair graphene nanoribbons (AGR) with long-range correlation between quantum wire contacts is investigated based on the tight binding model.
A metal–insulator transition is induced by disorder in neutral AGR. Therein, the conductance is one conductance quantum for the metallic phase and exponentially decays otherwise, when the length approaches to infinity and is far longer than the width. Similar to the case of long-range disorder, the conductance of neutral AGR first increases and then decreases while the conductance of doped AGR monotonically decreases, as the disorder strength increases. In the presence of strong disorder, the conductivity depends monotonically and non-monotonically on the aspect ratio for heavily doped and slightly doped AGR, respectively. For edge disordered graphene nanoribbons, the conductance increases monotonically and non-monotonically on the aspect ratio for longer than the width. Similar to the case of long-range correlated disorder while no delocalization occurs, since localization is induced by the edge disorder.

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