Effects of Hopping Modulation at the Edges on Transport Properties of Zigzag Graphene Nanoribbon Attached to Two Normal Metals

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Abstract. Transport properties of the junction composed of graphene nanoribbon with zigzag shaped edges attached to two normal metals are theoretically investigated. In order to clarify roles of zigzag edges on the transport properties, we consider the system where the hopping at the zigzag edges are weaker than the other bond. The results are compared with the case without modulation studied previously.

1. Introduction and model
A graphene nanoribbon (GNR) is a nanometer size graphene fragment and has been extensively studied as a new type of quasi one-dimensional electron systems. One of the most striking properties of the material is the feature that the shape of edges affects the electronic structure significantly[1, 2, 3]. In the case of armchair type edges, whether the system is metallic or insulating is dependent on the width of ribbon. On the other hand, the band structure of graphene nanoribbon with zigzag shaped edges, which is abbreviated to zigzag GNR in the following, is metallic irrespective of the width of ribbon N in the sense that the gap does not appear at the Fermi energy \( E = 0 \). The dispersion relation close to \( E = 0 \) does depend on \( N \) as \( E \propto \pm|k - \pi/a|^N \) where \( a \) expresses the lattice spacing. Such a singular dispersion relation is closely related to the fact that the states at the vicinity of \( E = 0 \) are well localized around the zigzag edges.

In the previous study, we have investigated transport properties of the junction composed of zigzag GNR attached to two normal metals (see Fig. 1)[4, 5], and obtained the following characteristic properties. The asymptotic behavior of the conductance at \( E = 0 \) for \( N_L \gg 1 \) depends on the parity of the width \( N \), where \( 2N_L \) expresses the length of GNR region of the junction. Namely, the quantity is proportional to \( N_L^{-2} \) for \( N = \text{even} \), whereas it tends to unity for \( N = \text{odd} \). In the presence of doping, we observe the conductance oscillation as a function of \( N_L \), which originates from interference between electron waves, but it disappears close to \( E = 0 \).

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In order to clarify roles of zigzag edges on the transport properties shown above, in the present study, we explore the transport properties in the case where the electron hopping at the
zigzag edges are weaker than the other bond. The model we consider is schematically shown in Fig. 1, where the zigzag GNR is sandwiched by the normal metals expressed by the regular square lattices. The hopping at the bonds written by the solid lines in both zigzag GNR and normal metal regions has the value, \( t \). At the zigzag edges in the GNR region, the hopping at the bond written by the dashed line and that by dotted one is given by \( c \times t \) and \( c' \times t \), respectively, where both \( c \) and \( c' \) are less than unity. Figure 1 (b) shows the square lattice-like model which is topologically equivalent to the present model of Fig. 1 (a). In Fig. 1 (b), the hopping in the cell vanishes alternatively. Therefore, we can extend the method developed in Ref. [7] to the present system in order to calculate the conductance \( g \) in unit of \( 2e^2/h \) (\( -e < 0 \) : electronic charge, \( h \) : Planck constant),
\[
g = \sum_{\mu,\nu} T_{\mu,\nu},
\]
where \( T_{\mu,\nu} \) is the transmission probability from the incident \( \nu \)-th channel to the transmitted \( \mu \)-th one, and can be obtained from the recursive Green’s function.

2. Results
In this section, we discuss the results obtained in the present study. The conductance at \( E = 0 \) and close to \( E = 0 \) as a function of \( N_L \), and the channel filtering seen in the transmission probability are investigated.

2.1. Conductance at \( E = 0 \) and close to \( E = 0 \)
At first, we discuss the conductance at \( E = 0 \) as a function of \( N_L \). Figure 2 show the conductances for the width \( N = 4 \) (a), \( N = 6 \) (b), \( N = 3 \) (c) and \( N = 5 \) (d). In each figure, solid, dotted and dashed curves express the case of hopping modulation at the zigzag edges as \( c = c' = 1.0 \), \( c = 0.5 \), \( c' = 1.0 \) and \( c = c' = 0.5 \), respectively. As is easily seen, the asymptotic value of the conductance for \( N_L \gg 1 \) in the presence of the hopping modulation \( (c, c' \neq 1) \) is the same as that in the case of \( c = c' = 1 \). It should be noted that this result is different from the \( N = 2 \) case[6];
\[
g^{N=2}(c,c') \simeq \frac{3}{N_L^2}(c^2 + c'^2).
\]
Figure 2. Conductance $g$ at $E = 0$ as a function of $N_L$ for the width $N = 4$ (a), $N = 6$ (b), $N = 3$ (c) and $N = 5$ (d). In each figure, solid, dotted and dashed curves express the case of $c = c' = 1.0$, $c = 0.5$, $c' = 1.0$ and $c = c' = 0.5$, respectively.

It may be because the zigzag GNR with the width $N = 2$ has a structure that it is composed of only the zigzag edges. In the case of $E \neq 0$, the conductance shows oscillation as a function of $N_L$ and the oscillation disappears close to $E = 0$ as is observed in $c = c' = 1$. In the region of vanishing oscillation, the value of the conductance is independent of the choice of $c$ and $c'$ except for $N = 2$. Thus, except the special case of $N = 2$, the asymptotic value of the conductance for $N_L \gg 1$ at the vicinity of $E = 0$ is independent of the choice of $c$ and $c'$.

2.2. Channel filtering and its breakdown

In the presence of the reflection symmetry in the transverse direction, the wave function in the direction is given by either even or odd function. Since the wave function of the normal metal region at the transverse direction is given by

$$u_{\nu}(l) = \sqrt{\frac{2}{N+1}} \sin \frac{\nu \pi}{N+1} l, \quad (\nu = 1, 2, \cdots, N)$$

the parity of the wave function is positive (negative) for the odd (even) channel number. On the other hand, in the zigzag GNR region with $N = \text{even}$ which possesses the reflection symmetry, the wave function for conduction (valence) band has positive (negative) parity[8, 9]. As a result, in the case of $E/t > 0$, only the transmission from the odd channel to the odd channel is possible, except in the vicinity of $E = 0$, where $T_{e,e}$ as well as $T_{o,o}$ remains finite with $e$ ($o$) being the even (odd) channel number. Such a filtering and its breakdown is observed for $c = c' = 0.5$ because the reflection symmetry is not broken as is seen in Fig 3 (a). According to Fig 3 (b) with $c = 0.5$, $c' = 1$ without reflection symmetry, except $E/t \approx 0$, all the transmission processes are allowed and the filtering does not occur. However, in the energy region close to $E \approx 0$, the processes from the incident channel with odd parity to the outgoing one with even parity and vice versa are forbidden and behavior of the transmission probabilities are the same as those with the reflection symmetry.
Figure 3. Transmission probability $T_{\mu,\nu}$ from the incident $\nu$-th channel to the outgoing $\mu$-th one for $E \gtrsim 0$, $N = 4$ and $N_L = 200$ together with the conductance $g$ as a function of $2k_F L/\pi$. The parameters of the hopping modulation, $c = c' = 0.5$ (a) and $c = 0.5, c' = 1$ (b) are used. The right end of the horizontal axis $2k_F L/\pi = 401$ corresponds to $E = 0$ in each figure. The quantities $T_{e,o}$ and $T_{o,e}$ express the transmission probability from the odd channel number to the even one and vice versa, respectively.

3. Summary
In the present paper, we investigated the transport properties of normal metal - zigzag GNR - normal metal junction. The hopping integral at the zigzag edges were modulated as $c \times t$ and $c' \times t$ ($c, c' < 1$) in order to clarify roles of zigzag edges on the transport properties. We found that the transport properties in the vicinity of $E = 0$ for $N_L \gg 1$ is independent of the choice of $c$ and $c'$ except for the $N = 2$ case. The results seem to indicate that the zigzag edges do not contribute to the transport properties of the present junction in such an interesting asymptotic region.

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