Selective Scattering in a Zigzag Graphene Nanoribbon

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Abstract. Electric transport of a zigzag graphene nanoribbon through a step-like potential or a potential barrier is studied by using the recursive Green’s function method. The results for a step-like potential show that scattering processes in a zigzag graphene nanoribbon obey a following selection rule: when the number of zigzag chains \( N \) is even, electrons in the band \( m \) are only scattered into the bands \( m + 2n \), where \( n \) is an integer. According to this selection rule, a step-like potential blocks the current when the potential height exceeds the incident energy as long as only the low-energy region is treated. Then, replacing a step-like potential with a potential barrier, we also show that it can play the role of a “band-selective filter”.

1. Introduction
Graphene, a single layer of carbon atoms, has various characteristic transport properties. Interestingly, electrons in a certain band behave as if they were massless relativistic particles [1], and thus can pass a potential barrier of any height. This effect is known as the Klein paradox [2], which enhances the conductivity of graphene. However, these transport properties change drastically for a zigzag graphene nanoribbon (Z-GNR), a long and narrow graphene strip with zigzag edges. Its band structure has well-separated valleys (conically-shaped curves) \( K \) and \( K' \). Furthermore, low-energy bands (the lowest conduction band and the highest valence band) form flat bands accompanied by the formation of the edge states [3]. In the case of a Z-GNR, a potential barrier blocks the current when the barrier height \( V_0 \) exceeds the incident energy \( E \) as long as the low-energy region including only the two low-energy bands is treated [4]. Since intervalley scatterings require substantial changes of momenta, they may be negligible. If this idea is applicable, then the sign of the group velocity should change when electrons enter the potential region, and thus they cannot penetrate the potential barrier. At first the current blocking caused by the potential barrier was interpreted in this way, but recently Akhmerov et al. showed theoretically that such a potential is a source of intervalley scatterings [6]. Thus, there must be another mechanism.

It is the purpose of the present study to clarify the mechanism for the current blocking. In the past studies of this phenomenon [4, 6], only the low-energy region has been treated. Besides them, we consider the case of the higher incident energies, and discuss in more detail how electrons are scattered by a step-like potential. As is shown in Sec. 2, the results imply that scattering processes in a Z-GNR obey a selection rule for the band indices. According to the selection rule, scattering processes between the low-energy bands are strictly suppressed. Thus, as long as only the low-energy region is treated, this suppression should give rise to the current...
Figure 1. (a) A schematic diagram of a Z-GNR with a potential step given in Eq. (3). The x-axis (y-axis) is taken in perpendicular (parallel) to graphene leads. $N$ denotes the number of zigzag chains. (b) Schematic diagrams of a band structure of a Z-GNR. The bands are indexed as shown in the diagram.

blocking mentioned above. In Sec. 3, it is shown that a potential barrier plays the role of a “band-selective filter”. The summary is given in Sec. 4.

2. The step-like potential
In this paper, we describe the electronic states of a Z-GNR with a finite width $N$ (see Fig. 1(a)) by the tight-binding Hamiltonian

$$ H = - \sum_{i,j} \tau_{ij} |i\rangle \langle j| + \sum_i V_i |i\rangle \langle i|. $$

(1)

The hopping integral $\tau_{ij} = \tau$ when $i$ and $j$ are nearest neighbor sites, and $\tau_{ij} = 0$ otherwise. $V_i = V(\mathbf{r}_i)$ is the electrostatic potential energy on the site $i$. The zero-bias conductance of a Z-GNR is determined by the multi-channel Landauer formula

$$ G = \frac{2e^2}{h} \sum_{\mu,\nu} T(\mu, \nu), \quad T(\mu, \nu) = |t_{\mu\nu}|^2, $$

(2)

where the summation runs over all incoming ($\nu$) and outgoing ($\mu$) channels, $t_{\mu\nu}$ is a transmission coefficient, and $T(\mu, \nu)$ represents a transmission probability. In order to calculate $t_{\mu\nu}$, the recursive Green’s function method [7] is adopted. Here we specify $\nu$ ($\mu$) by the valley and band indices, e.g., the transmission probability of the scattering process from the incoming channel in the band 0 belonging to valley $K$ into the outgoing channel in the band $-2$ belonging to valley $K'$ is denoted by $T(K_0', K_0)$ (see Fig. 1(b)).

In this section, we consider the effect of a potential step described as

$$ V(\mathbf{r}) = V(y) = V_0 \Theta(y), \quad \Theta(y) = \begin{cases} 0 & (y < -2d), \\ \frac{1}{2} \left[ \tanh(2y/d) + 1 \right] & (|y| \leq 2d), \\ 1 & (y > 2d). \end{cases} $$

(3)

In the present calculation, we set $d = 10a$ ($a$ is the lattice constant), and the incident energy is fixed at $E = 0.5\tau$ while $V_0$ is varied from 0 to $\tau$. The transmission probabilities are obtained as a function of $\varepsilon = E - V_0$.

The results for $N = 30$ are shown in Fig. 2(a). The electrons in the band 0 are scattered only into the bands 0, $\pm2$, and $\pm4$. Similarly, the electrons in the band 1 are scattered only into
the bands ±1, ±3, and −5. These results show that scattering processes in a Z-GNR obey a following selection rule: the electrons in the band \(m\) are only scattered into the bands \(m + 2n\), where \(n\) is an integer in the range \([-\frac{N + m}{2}, \frac{N - m - 1}{2}]\).

Now, we reconsider the interpretation of the current blocking for the case where the incident energy \(E\) crosses only the two low-energy bands. When \(E > V_0\), the electrons in the band 0 can transmit through a step-like potential because they can be scattered into the band 0. Though, when \(E < V_0\), they must be reflected because they cannot be scattered into the band −1 according to the selection rule.

Fig. 2(b) shows the results for \(\nu = K_0\) and \(N = 31\). When \(N\) is odd, the selection rule does not exist. This results do not conflict with the results shown in Ref. [6].

3. The potential barrier
Since our potential barrier consists of two step-like potentials, scattering processes caused by it also obey the selection rule when \(N\) is even, and thus the potential barrier plays the role of a “band-selective filter”. To show this, we redefine \(V(\vec{r})\) as

\[
V(\vec{r}) = V(y) = V_0[\Theta(y) - \Theta(y - L)],
\]

and introduce following quantities

\[
P_{\text{even}} = \frac{\sum_{\mu, \nu} T(\mu, \nu)}{\sum_{\mu, \nu} T(\mu, \nu)}, \quad P_{\text{odd}} = \frac{\sum_{\mu, \nu} T(\mu, \nu)}{\sum_{\mu, \nu} T(\mu, \nu)}, \quad P_{\text{even}} + P_{\text{odd}} = 1,
\]

where \(\mu_{\text{even}}\) (\(\mu_{\text{odd}}\)) represents the outgoing channels with even (odd) index.

The results of the calculations are shown in Fig. 3. In the light gray region, \(\varepsilon\) crosses only the band 0 in the potential region (see Fig. 4), thus \(P_{\text{even}}\) becomes 1 and \(P_{\text{odd}}\) becomes 0 due to the selection rule. Similarly, in the dark gray region, \(\varepsilon\) crosses only the band −1 in the potential region, thus \(P_{\text{odd}}\) becomes 1 and \(P_{\text{even}}\) becomes 0. This means that a potential barrier in a

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**Figure 2.** (a) The transmission probabilities for \(\nu = K_0\) and \(\nu = K_1\) with \(N = 30\). Since \(T(K_0', K_0), T(K_1, K_0), T(K_1', K_0)\) and \(T(K_0', K_1')\) have a non-zero yet very small value (\(<10^{-5}\)) respectively, we do not show them in the diagram. The others (\(T(K_1, K_0), T(K_2, K_1), \) etc.) are strictly suppressed to 0. (b) The transmission probabilities for \(\nu = K_0\) and \(N = 31\).
Figure 3. The results of the calculations of $P_{\text{even}}$ and $P_{\text{odd}}$. In the light (dark) gray region, $P_{\text{even}}$ ($P_{\text{odd}}$) becomes 1 and $P_{\text{odd}}$ ($P_{\text{even}}$) becomes 0.

Z-GNR plays the role of a band-selective filter. That is to say, when $V_0$ is chosen for $\varepsilon$ to be in the light (dark) gray region, the potential barrier transmits only the electrons in the bands with even (odd) index.

4. Summary
We have studied electric transport of a Z-GNR through a step-like potential or a potential barrier by using the recursive Green’s function method. It has been shown that scattering processes in a Z-GNR obey the selection rule for the band indices when the number of zigzag chains $N$ is even. Due to this selection rule, a step-like potential blocks the current when $E < V_0$, as long as only the two lowest energy bands have main contributions. We have also shown that a potential barrier can play the role of the band-selective filter, which transmits only the electrons in the bands with either even or odd index depending on $\varepsilon = E - V_0$.

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References
[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 \textit{Nature} \textbf{438} 197
[2] Katsnelson M I, Novoselov K S and Geim A K 2006 \textit{Nature Phys.} \textbf{2} 620
[3] Nakada K, Fujita M, Dresselhaus G and Dresselhaus M S 1996 \textit{Phys. Rev. B} \textbf{54} 17954
[4] Wakabayashi K and Aoki T 2002 \textit{Int. J. Mod. Phys. B} \textbf{16} 4897
[5] Rycerz A, Tworzydlo J and Beenakker C W J 2007 \textit{Nature Phys.} \textbf{3} 172
[6] Akhmerov A R, Bardarson J H, Rycerz A and Beenakker C W J 2008 Theory of the valley-valve effect in graphene nanoribbons \textit{Preprint} cond-mat.mes-hall/0712.3233
[7] Ando T 1991 \textit{Phys. Rev. B} \textbf{44} 8017