Band-Selective Filter in a Zigzag Graphene Nanoribbon

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Electric transport of a zigzag graphene nanoribbon through a steplike potential and a barrier potential is investigated by using the recursive Green's function method. In the case of the steplike potential, we demonstrate numerically that scattering processes obey a selection rule for the band indices when the number of zigzag chains is even; the electrons belonging to the "even" ("odd") bands are scattered only into the even (odd) bands so that the parity of the wave functions is preserved. In the case of the barrier potential, by tuning the barrier height to be an appropriate value, we show that it can work as the "band-selective filter", which transmits electrons selectively with respect to the indices of the bands to which the incident electrons belong. Finally, we suggest that this selection rule can be observed in the conductance by applying two barrier potentials.

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Graphene, a single layer of graphite, is one of the most intriguing new materials, which has been studied vigorously since Novoselov *et al.* first succeeded in fabricating it in 2004 [1]. Particularly, its excellent transport properties such as the high mobility at room temperature have attracted a lot of research interest to apply it in making future electronic devices [2,3]. However, to realize graphene-based devices, there is a crucial problem: the characteristic gapless band structure makes the control of the electric current rather difficult. Many attempts to overcome this problem have been made so far, and have given rise to various beneficial systems such as a graphene quantum dot [4], epitaxial graphene on SiC substrates [5], and a graphene nanoribbon [6].

We shall focus on a graphene nanoribbon with zigzag edges [7] (hereafter we call it "zigzag ribbon"). A band structure of a zigzag ribbon has two well-separated valleys (conically-shaped curves) K and K' around the vertices of the first Brillouin zone. In addition, the low-energy bands (the lowest conduction band and the highest valence band) are almost flat at the Fermi level due to the edge states [6,7]. Such a peculiar band structure has motivated many researchers to investigate the electric transport of a zigzag ribbon. Wakabayashi and Aoki [8] found that the electric current is almost entirely blocked by a barrier potential when the incident energy E_I is in the range $[0, \Delta]$ while the barrier height V_0 is in the range $[\Delta, 2\Delta]$ [2Δ is the energy separation between the top of the next highest valence band and the bottom of the next lowest conduction band; see Fig. 1(a)]. This result is quite different from the case of bulk graphene, where incident electrons in the low-energy bands can pass a barrier potential of any height (known as the Klein paradox [9]). At first, the polarization of two valleys was considered to be the origin of this current blocking effect, and then it was named the "valley-valve effect" [10] by using an analogy from the spin-valve effect [11]. In a recent study [12], however, Akhmerov *et al.* pointed out that the origin is not the valley polarization and showed that the behavior of the conductance is strongly connected with the parity of the number of zigzag chains N.

This striking current blocking effect has the possibility to control the electric current. In this Letter, we investigate the role of a barrier potential applied to a zigzag ribbon in more detail, and suggest the way to control the current in a

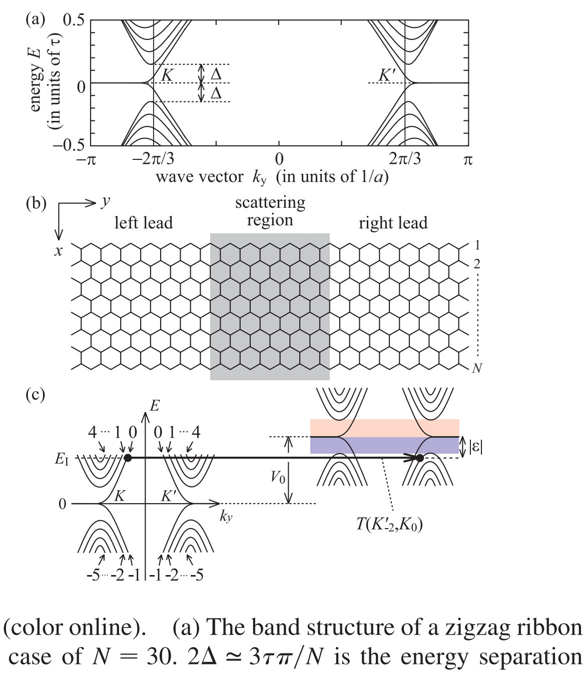

FIG. 1 (color online). (a) The band structure of a zigzag ribbon for the case of $N = 30$. $2\Delta \simeq 3\tau\pi/N$ is the energy separation between the top of the next highest valence band and the bottom of the next lowest conduction band. (b) A schematic diagram of a zigzag ribbon. The electrostatic potential varies in the shaded region. The x axis (y axis) is taken to be perpendicular (parallel) to graphene lead lines. (c) A schematic diagram of the scattering process from K_0 into K'_{-2} (see text). The bands are indexed as shown in the diagram. The colored regions shown in the diagram correspond to the ones shown in Figs. 4 and 5.

new light. The single-orbital tight-binding model is employed to describe the electronic states of a zigzag ribbon. The Hamiltonian is written as $H = -\sum_{i,j}\tau_{ij}|i\rangle\langle j| + \sum_i V(y_i)|i\rangle\langle i|$, where the hopping integral $\tau_{ij} = \tau$ when i and j are nearest neighbor sites, and $\tau_{ij} = 0$ otherwise. $V(y_i)$ is the electrostatic potential energy applied at the site i, which varies only along the direction of graphene lead lines [see Fig. 1(b)]. The zero-bias conductance from the left lead to the right lead is given by the Landauer formula [13] $G = \frac{2e^2}{h}\sum_{\mu,\nu}T(\mu,\nu)$, where the summation runs over all incoming (ν) and outgoing (μ) channels, $T(\mu,\nu) = |t_{\mu\nu}|^2$ represents a transmission probability, and $t_{\mu\nu}$ is a transmission coefficient. We specify channels ν and μ by the valley and band indices; the right-moving channel in the band n belonging to the valley K (K') is denoted by K_n (K'_n). For example, the transmission probability of the scattering process from the incoming channel in the band "0" belonging to the valley K into the outgoing channel in the band "-2" belonging to the valley K' is denoted by $T(K'_{-2}, K_0)$ [see Fig. 1(c)]. Hereafter we call bands with even (odd) indices "even" ("odd") bands. For the calculation of the transmission coefficients, we adopt the recursive Green's function method developed by Ando [14,15].

A steplike potential.—Now, we consider the effect of a smooth steplike potential described as

$$V(y) = V_0\Theta(y), \tag{1}$$

$$\Theta(y) = \begin{cases} 0 & (y < -d), \\ (1/2)[\sin(\pi y/2d) + 1] & (|y| \le d), \\ 1 & (y > d). \end{cases} \tag{2}$$

In the present calculation, we set $d = 10a$ (a is the lattice constant) and the incident energy is fixed at $E_I = 0.5\tau$ while V_0 is varied from 0 to τ. The transmission probabilities are obtained as a function of $\varepsilon = E_I - V_0$. From the results, we find that scattering processes caused by the steplike potential obey the following selection rule: the electrons in the even (odd) bands can be scattered only into the even (odd) bands and other scattering processes are entirely restricted. For example, Figs. 2(a) and 2(b) show the transmission probabilities for $\nu = K_0$ and $\nu = K_1$ with $N = 30$. The electrons in the band 0 are scattered only into the bands 0, ± 2, and ± 4. Similarly, the electrons in the band 1 are scattered only into the bands ± 1, ± 3, and -5.

The origin of this selection rule is the conservation of the parity of wave functions [16–20]. As is shown in Fig. 3(a), a zigzag ribbon has the reflection symmetry with respect to $x = 0$ line when N is even. Thus, wave functions must be either even or odd functions of x. For example, as is shown in Figs. 3(b) and 3(c), the wave functions of the incoming channel K_0 and the outgoing channels K_{-2} and K_{-4} are even functions, while the incoming channel K_1 and the outgoing channels K'_{-1} and K_{-3} are odd functions. Similarly, other wave functions for even (odd) bands are even (odd) functions. Since the steplike potential given in

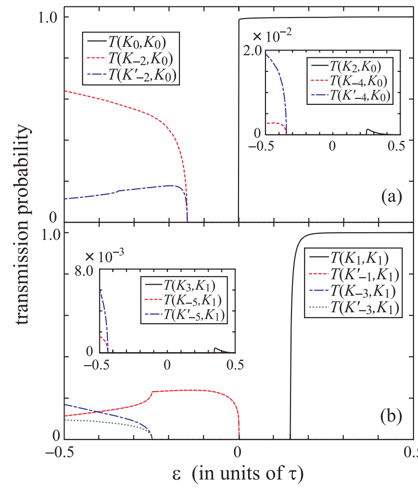

FIG. 2 (color online). The transmission probabilities for (a) $\nu = K_0$ and (b) $\nu = K_1$ with $N = 30$. The insets are the enlargements of the low-probability regions. Although we do not show $T(K'_2, K_0)$, $T(K_4, K_0)$, $T(K'_4, K_0)$ and $T(K'_3, K_1)$ in the diagram, they have a very small yet nonzero value (less than $\sim 10^{-4}$), respectively. The others ($T(K_1, K_0)$, $T(K_2, K_1)$, etc.) are suppressed to 0. It can be seen that intravalley scatterings are not always dominant compared to intervalley scatterings, e.g., $T(K_4, K_0) < T(K'_4, K_0)$.

Eq. (1) cannot change the parity of wave functions, only the scattering processes which preserve the parity of wave functions can occur. Thus, the transmission probabilities such as $T(K_{-2}, K_0)$ have nonzero values and the ones such

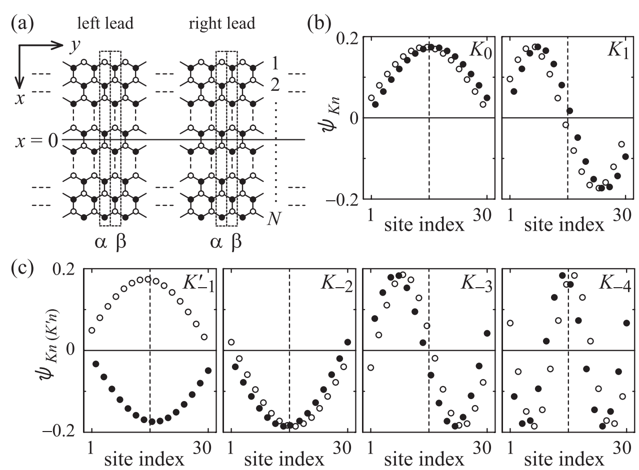

FIG. 3. (a) A schematic diagram of a zigzag ribbon for even N. Open and filled circles represent two inequivalent sublattices, respectively. One can regard a zigzag ribbon as a quasi-one-dimensional system. In this regime, the columns α and β are treated as quasi sublattices. (b),(c) The wave functions can be written as $\Psi_{K_n(K'_n)}(x,y) = \psi_{K_n(K'_n)}(x)e^{ik_y y}$. We show $\psi_{K_n(K'_n)}(x)$ of (b) the incoming channels K_0, K_1 on the quasi sublattice α in the left lead for $E_I = 0.5\tau$, (c) the outgoing channels K'_{-1}, K_{-2}, K_{-3} and K_{-4} on α in the right lead for $\varepsilon = -0.5\tau$. The wave functions on the quasi sublattice β have the same parity as the one of the wave functions on α. Here $N = 30$.

as $T(K'_{-1}, K_0)$ are restricted to 0 [see Figs. 2(a) and 2(b)]. On the other hand, when N is odd, a zigzag ribbon does not have the reflection symmetry and wave functions are neither an even nor odd function of x. Consequently, the selection rule does not exist in this case.

Barrier potentials.—By calculating the transmission probabilities individually, we have just shown that scattering processes obey the selection rule when N is even. However, the existence of the selection rule shown in Figs. 2(a) and 2(b) cannot be ascertained in experiments because the conductance is proportional to the sum of all transmission probabilities. Now, we show that the existence of the selection rule can be observed in the conductance by applying two barrier potentials.

First, we consider the case of one barrier potential

$$V(y) = V_0[\Theta(y) - \Theta(y - L_0)]. \tag{3}$$

To see the role of this potential, we introduce the following quantities:

$$P_e = \frac{\sum_{\mu_e,\nu} T(\mu_e, \nu)}{\sum_{\mu,\nu} T(\mu, \nu)}, \qquad P_o = 1 - P_e = \frac{\sum_{\mu_e,\nu} T(\mu_e, \nu)}{\sum_{\mu,\nu} T(\mu, \nu)}, \tag{4}$$

where μ_e (μ_o) represents the outgoing channels with even (odd) index. The results of the calculations are shown in Fig. 4. We can see at once that some plateaus appear when $\varepsilon > 0$. In this region, the contributions of the transmission probabilities of the scattering processes between the same channels ($T(K_0, K_0)$, $T(K_1, K_1)$, etc.) are major ($\simeq$1) and the others are minor ($\lesssim 10^{-3}$) (see Fig. 2). Thus, P_e and P_o are given as $P_e \simeq \mathcal{N}_e/\mathcal{N}$ and $P_o \simeq \mathcal{N}_o/\mathcal{N}$, respectively. Here $\mathcal{N}_e$ ($\mathcal{N}_o$) represents the number of the right-moving channels with even (odd) index in the potential region, and $\mathcal{N} = \mathcal{N}_e + \mathcal{N}_o$.

Let us focus on the behavior in the colored regions shown in the diagram. In the red (or light gray) region (hereafter called the "even-pass region"), ε crosses only the band 0 [see Fig. 1(c)], and thus $P_e \simeq 1$ and $P_o \simeq 0$ due to the selection rule [21]. In contrast, in the blue (or dark gray) region (hereafter called the "odd-pass region"), ε crosses only the band -1, and thus $P_o \simeq 1$ and $P_e \simeq 0$. These results mean that a barrier potential in a zigzag ribbon plays the role of a "band-selective filter": when ε is tuned to be in the even (odd) pass region, the barrier potential transmits only the electrons in the even (odd) bands.

The dashed lines in Fig. 4 denote the results in the presence of the Anderson disorder potential $V_{\rm imp}(\boldsymbol{r}_i) = \sum_{\boldsymbol{r}_m}^{\rm (random)} U_m \delta_{\boldsymbol{r}_i,\boldsymbol{r}_m}$. Here we assume that the impurities are uniformly distributed with a strength $U_m \in [-\tau/2, \tau/2]$ and a density $n = 0.01$. As can be seen, the quality of the band-selective filter is still excellent in such a disordered system.

Next, we append one more barrier potential to the system as follows:

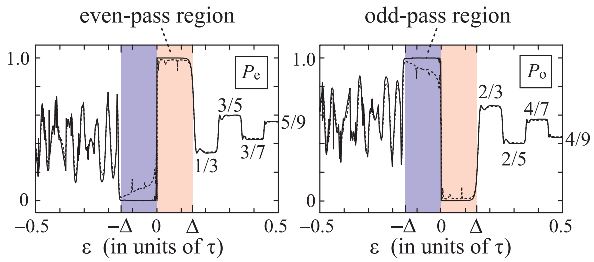

FIG. 4 (color online). P_e and P_o for the clean system (solid line) and the disordered system (dashed line) with $L_0 = 50a$. The impurities are distributed in the range $y \in [-50a, 100a]$ and each dashed line is an average over 10 realizations of random potentials. The integral ratios shown in the left (right) panel represent the values of $\mathcal{N}_e/\mathcal{N}$ ($\mathcal{N}_o/\mathcal{N}$) (see text). The colored regions shown in the diagram correspond to the ones shown in Fig. 1(c).

$$V(y) = V_0[\Theta(y) - \Theta(y - L_0)] + V'[\Theta(y - L_0 - L_1) - \Theta(y - L_0 - L_1 - L_2)], \tag{5}$$

where V_0 is fixed so that the first barrier potential behaves as the band-selective filter (i.e., $|E_I - V_0| \leq \Delta$), and V' is varied from 0 to τ. Introducing two barrier potentials like that, one can observe the existence of the selection rule in the conductance. For example, when ε is tuned to be in the even-pass region, the first potential works as the band-selective filter which transmits only the electrons in the even bands. In this case, since the incident electrons in the odd bands are reflected by this band-selective filter, all the electrons after passing the first potential belong to the even bands. Then, one can ignore the odd bands in the second potential because the scattering processes from even bands into odd bands are restricted by the selection rule. This indicates that the odd-pass region in the second potential turns to the pseudogap region [see Fig. 5(a); the negligible odd bands are shown as dashed lines]. In fact, as is shown in the left panel of Fig. 5(b), the conductance of the clean system is entirely suppressed when $\varepsilon' = E_I - V'$ is in the odd-pass (pseudogap) region. Similarly, when ε is tuned to be in the odd-pass region, the even-pass region in the second potential turns to the pseudogap region [see the right panel of Fig. 5(b)]. We note that the conductance of the disordered system is also suppressed in the pseudogap region, although the leak current slightly increases.

Recently, Rycerz *et al.* [10] calculated the valley polarization of the current transmitted through a barrier potential, and showed that the transmitted current can be polarized in one of two valleys by tuning the height of the potential. This means that a barrier potential may be used as a "valley filter". They demonstrated the operation of the valley filter in the cases where the potential changes abruptly and smoothly. According to the results, however, the quality of the valley filter is somewhat poor in both cases when $E_I < V_0$, and especially in the case of a smooth potential the decline is severe (see Fig. 4 of Ref. [10]). In contrast, whether the potential change is abrupt or smooth,

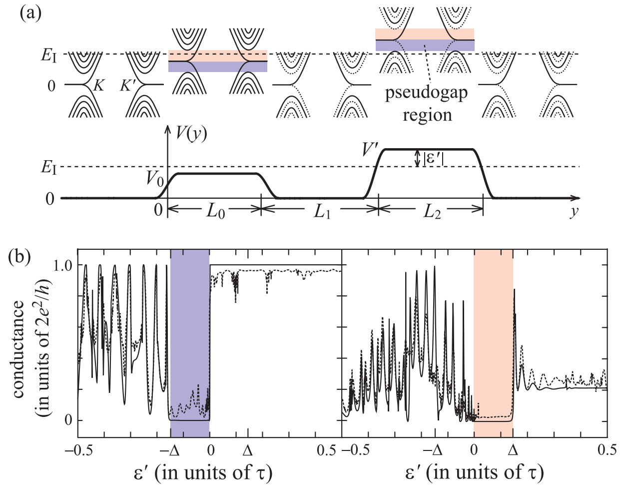

FIG. 5 (color online). (a) Schematic diagrams of band structures and the barrier potential described as Eq. (5). (b) The conductances for the clean system (solid line) and the disordered system (dashed line) with $L_0 = L_2 = 50a$ and $L_1 = 100a$. The impurities are distributed in the range $y \in [-50a, 250a]$ and each dashed line is an average over 10 realizations of random potentials. In the left (right) panel, V_0 is tuned to be 0.426τ (0.574τ) so that ε is in the even (odd) pass region, and thus the odd (even) pass region in the second potential turns to the pseudogap region. In the region $\varepsilon' < 0$, only interband scatterings occur, which makes the behavior of the conductances complicated.

and even in the presence of disorder, the quality of the band-selective filter we have suggested here is sufficiently high even in the region $E_I < V_0$.

Here we discuss the feasibility of an experiment to confirm these parity effects. In recent years, process technologies for making graphene-based devices have made rapid strides. Particularly, local electrostatic gates [22] and only sub-10 nm wide ($N \simeq 10$) graphene nanoribbon field-effect transistors [23] are already realized in experiments. Thus, if an edge shape of a graphene nanoribbon can be controlled, then one can confirm the parity effects in experimental results. Very recently, Koskinen *et al.* predicted that zigzag edges are thermodynamically metastable and hexagonal rings should be reconstructed into pentagonal and heptagonal rings [24]. Even in this case, the parity effects survive because the relation between band indices and parity of wave functions do not change [25]. We thus expect that it will be possible to carry out an experiment and to confirm the parity effects in the near future.

In summary, we have studied electric transport of a zigzag ribbon through a steplike potential or a barrier potential by using the recursive Green's function method. It has been shown that scattering processes in a zigzag ribbon obey the selection rule for the band indices when the number of zigzag chains N is even. Moreover, we have also shown that a barrier potential 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 $\varepsilon = E_I - V_0$. Finally, we have suggested that the selection rule can be observed in the conductance by applying two barrier potentials to a graphene ribbon.

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[1] K. S. Novoselov *et al.*, Science **306**, 666 (2004).
[2] Y. B. Zhang *et al.*, Nature (London) **438**, 201 (2005).
[3] A. K. Geim and K. S. Novoselov, Nature Mater. **6**, 183 (2007).
[4] B. Trauzettel *et al.*, Nature Phys. **3**, 192 (2007).
[5] S. Y. Zhou *et al.*, Nature Mater. **6**, 770 (2007).
[6] K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B **54**, 17 954 (1996).
[7] M. Fujita *et al.*, J. Phys. Soc. Jpn. **65**, 1920 (1996).
[8] K. Wakabayashi and T. Aoki, Int. J. Mod. Phys. B **16**, 4897 (2002).
[9] M. I. Katsnelson *et al.*, Nature Phys. **2**, 620 (2006).
[10] A. Rycerz, J. H. Bardarson, A. Rycerz, and C. W. J. Beenakker, Nature Phys. **3**, 172 (2007).
[11] A. Wolf *et al.*, Science **294**, 1488 (2001).
[12] A. R. Akhmerov, J. H. Bardarson, A. Rycerz, and C. W. J. Beenakker, Phys. Rev. B **77**, 205416 (2008).
[13] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); M. Buttiker, Phys. Rev. Lett. **57**, 1761 (1986).
[14] T. Ando, Phys. Rev. B **44**, 8017 (1991).
[15] K. Wakabayashi, Doctoral thesis, University of Tsukuba, 2000.
[16] J. Nakabayashi and S. Kurihara, J. Phys. Conf. Ser. (to be published).
[17] A. Cresti, G. Grosso, and G. P. Parravicini, Phys. Rev. B **77**, 233402 (2008).
[18] D. Rainis *et al.*, arXiv:0806.4475.
[19] There are similar discussions on the selection rule in Ref. [18]. Our previous work, Ref. [16] (submitted on 13/06/2008), and the present work are done independently of their work.
[20] In the case of the extreme limit $N = 2$ (namely the case of polyacene), this parity effect was discussed analytically in the following paper: N. M. R. Peres and F. Sols, J. Phys. Condens. Matter **20**, 255207 (2008).
[21] Actually the value of P_e (P_o) is not strictly 1 (0) because of the tunneling effect.
[22] B. Özyilmaz *et al.*, Phys. Rev. Lett. **99**, 166804 (2007).
[23] X. Wang *et al.*, Phys. Rev. Lett. **100**, 206803 (2008).
[24] P. Koskinen, S. Malola, and H. Hakkinen, Phys. Rev. Lett. **101**, 115502 (2008).
[25] J. Nakabayashi, D. Yamamoto, and S. Kurihara (unpublished).