Electronic Transport Properties of Disordered Graphene Nanoribbons

Katsunori Wakabayashi¹², Yositake Takane¹, and Manfred Sigrist³

¹Department of Quantum Matter, Hiroshima University, Higashi-Hiroshima 739-8530, Japan
²PRESTO, Japan Science and Technology Agency (JST), Kawaguchi 332-0012, Japan
³Theoretische Physik, ETH-Hönggerberg, Zürich CH-8093, Switzerland

E-mail: kwaka@hiroshima-u.ac.jp

Abstract. The band structure of graphene ribbons with zigzag edges have two valleys well separated in momentum space, related to the two Dirac points of the graphene spectrum. The propagating modes in each valley contain a single chiral mode originating from a partially flat band at band center. This feature gives rise to a perfectly conducting channel in the disordered system, if the impurity scattering does not connect the two valleys, i.e. for long-range impurity potentials. We extend our analysis for the case of nanoribbons with general edge structures.

1. Introduction

The successive fabrication of graphene devices [1] has has initiated intensive and diverse research on carbon related systems. The honeycomb crystal structure of single layer graphene consists of two inequivalent sublattices and results in a unique band structure for the itinerant \(\pi\)-electrons near the Fermi energy which behave as massless Dirac fermion. In graphene, the presence of edges can have strong implications for the spectrum of the \(\pi\)-electrons. [2, 3] In graphene nanoribbons with zigzag edges, localized states appear at the edge with energies close to the Fermi level. [2, 3] In contrast, edge states are absent for ribbons with armchair edges. Recent experiments give evidence for edge localized states. [4] Also graphene nanoribbons are synthesized using lithography techniques [5] and chemical techniques. [6]

The electron transport in 1-dimensional (1D) carbon systems displays unusual properties, in apparent conflict with the common belief that 1D systems are generally subjected to Anderson localization. Indeed it was demonstrated that carbon nanotubes with long-ranged impurities possess one perfectly conducting channel (PCC) [7]. Recently we have pointed out that zigzag nanoribbons with long ranged impurities (LRI) also possess such PCC due to the chiral mode originating graphene edge states. [8] Here we discuss the electronic transport properties of graphene nanoribbon with LRIs using Landauer approach.

We describe the electronic states of nanographites by the tight-binding model

\[
H = \sum_{i,j} \gamma_{i,j} |i\rangle\langle j| + \sum_i V_i |i\rangle\langle i|,
\]

where \(\gamma_{i,j} = -1\) if \(i\) and \(j\) are nearest neighbors, and \(0\) otherwise. \(|i\rangle\) represents the state of the \(p_z\)-orbital on site \(i\) neglecting the spin degrees of freedom. In the following we will also apply...
Figure 1. (a) Structure of graphene zigzag ribbon. The disordered region with randomly distributed impurities lies in the shaded region and has the length $L$. The lattice constant is $a$ and the ribbon width $N$ is defined as the number of the zigzag chains. Randomly distributed blue circles schematically represent the long ranged impurities. (b) Energy dispersion of zigzag ribbon with $N = 20$. The valleys in the energy dispersion near $k = 2\pi/3a$ ($k = -2\pi/3a$) originate from the Dirac $K_+ (K_-)$-point of graphene. The red-filled (blue-unfilled) circles denote the right (left)-moving open channel at the energy $E_0$ (dashed horizontal line). In the left(right) valley, the degeneracy between right and left moving channels is missing due to one excess right(left)-going mode. The time-reversal symmetry under the intra-valley scattering is also broken. (c) $L$-dependence of the average $\langle g \rangle$ of dimensionless conductance for zigzag ribbon with $N = 20$, $d/a = 3.0$ (no inter-valley scattering), $u_0 = 0.1$, and $n_{\text{imp}} = 0.1$. More than 3000 samples with different impurity configuration are included in the ensemble average.

magnetic fields perpendicular to the graphite plane which are incorporated via the Peierls phase:

$$\gamma_{ij} \rightarrow \gamma_{ij} \exp \left[ i2\pi \frac{e}{\hbar} \int_{i}^{j} dl \cdot A \right],$$

where $A$ is the vector potential. The second term in Eq. (1) represents the impurity potential, $V_i = V(\mathbf{r}_i)$ is the impurity potential at a position $\mathbf{r}_i$.

As shown in Fig.1(a), our zigzag ribbons are characterized by the width $N$, the number of zigzag chains, and $L$ denotes the length of the disordered region. In Fig. 1(b), we display the band structure for the zigzag ribbon with $N = 20$. Note that zigzag ribbons are metallic for all widths at finite doping because of the presence of a partial flat band at zero energy induced by edge states. These edge states lead in the clean limit to the characteristic conductance odd-number quantization, i.e. $g = 2n+1$ as the dimensionless conductance per spin ($n = 0, \pm 1, \pm 2, \ldots$) [8, 9, 10]. There are two valleys, at $k_\pm = \pm 2\pi/3$, each of which possesses one excess mode which violates the balance between the number left- and right-moving modes (Fig.1).

In our model we assume that the impurities are randomly distributed with a density $n_{\text{imp}}$, and the potential has a Gaussian form of range $d$

$$V(\mathbf{r}_i) = \sum_{\mathbf{r}_0 \text{(random)}} u \exp \left( -\frac{|\mathbf{r}_i - \mathbf{r}_0|^2}{d^2} \right),$$

where the strength $u$ is uniformly distributed within the range $|u| \leq u_M$. Here $u_M$ satisfies the normalization condition: $u_M \sum_{\mathbf{r}_i} \exp \left( -\frac{r_i^2}{d^2} / \sqrt{3}/2 \right) = u_0$. The range of the impurity potential is crucial for the transport properties. Since the momentum difference between two valleys is rather large, $\Delta k = k_+ - k_- = 4\pi/3a$, only short-range impurities (SRI) with a range
smaller than the lattice constant causes inter-valley scattering. Long-range impurities (LRI), in contrast, restrict the scattering processes to intra-valley scattering [11].

Ignoring the true spins the graphene systems have the time reversal symmetry (TRS) with respect to the operator $T$ represented by the complex conjugation $\mathcal{C}$, pairs of time-reversed states are formed across the two valleys (Dirac points). In the absence of the inter-valley scattering due to the LRI, such total TRS becomes irrelevant. Then TRS restricted to each valley can be formulated as $T = -i(\sigma^y \otimes 1_2)\mathcal{C}$, where the A-B-sublattices act as pseudospin degrees of freedom. The boundary conditions which treat the two sublattices asymmetrically leading to edge states give rise to a single special mode in each valley. Considering now one of the two valleys separately, say the one around $k = k_+$ we see that the TRS is effectively violated in the sense that we find one more left-moving than right-moving mode. If we restrict ourselves to disorder promoting only intra-valley scattering, transport properties would resemble those of a system with a chiral mode which is oppositely oriented for the two valleys. In this sense such a system violates TRS. On the other hand, disorder yielding inter-valley scattering would restore this TRS as both valleys together incorporate a complete set of pairs of time-reversed modes. Thus we expect to see qualitative differences in the properties if the range of the impurity potentials is changed.

The dimensionless electrical conductance is calculated using the Landauer-Büttiker formula, $g(E) = \text{Tr}(tt^\dagger)$, where $t(E)$ is the transmission matrix through the disordered region. This transmission matrix can be calculated by means of the recursive Green function method. [9] Here we show the case of LRI using a potential with $d/a = 3.0$ which is already sufficient to avoid inter-valley scattering. Fig.1(c) shows the averaged dimensionless conductance as a function of $L$ for different incident energies, averaging over an ensemble of more than 4800 samples with different impurity configurations for ribbons of the width $N = 20$. The potential strength and impurity density are chosen to be $u_0 = 0.1$ and $n_{\text{imp.}} = 0.1$, respectively. As a typical localization effect we observe that $\langle g \rangle$ gradually decreases with growing length $L$. Interestingly, $\langle g \rangle$ converges to $\langle g \rangle = 1$, indicating the presence of a single perfectly conducting channel. It should be noted that $\langle g \rangle(L)$ has an exponential behavior as $\langle g \rangle \rightarrow 1 - \exp(-L/\xi)$ with $\xi$ as the localization length. The result for narrower ribbon can be found in former publication. [8]

As the effect is connected with the subtle feature of an excess mode in band structure, it is natural that the result can only be valid for sufficiently weak potentials. For potential strengths comparable to the energy scale of the band structure, e.g. the energy difference between the transverse modes, the result should be qualitatively altered[12].

As we have seen, zigzag ribbons with long-ranged impurity potentials retain a single PCC. This PCC originates for the following two reasons: (i) The spectrum contains two valleys (two Dirac $K_{\pm}$-points) which are well enough separated in momentum space as to suppress intervalley scattering due to the long-ranged impurities, (ii) the spectrum in each valley is chiral (two Dirac points) which are well enough separated in momentum space as to suppress inter-valley scattering due to the long-ranged impurities, (ii) the spectrum in each valley is chiral (two Dirac points) which are well enough separated in momentum space as to suppress inter-valley scattering due to the long-ranged impurities, (ii) the spectrum in each valley is chiral (two Dirac points) which are well enough separated in momentum space as to suppress inter-valley scattering due to the long-ranged impurities, (ii) the spectrum in each valley is chiral (two Dirac points) which are well enough separated in momentum space as to suppress inter-valley scattering due to the long-ranged impurities, (ii) the spectrum in each valley is chiral (two Dirac points) which are well enough separated in momentum space as to suppress inter-valley scattering due to the long-ranged impurities.

We extend our analysis to the electronic spectrum of nanoribbons for which the ribbon axis is tilted with respect to the zigzag axis and keep the balance between $A$- and $B$-sublattice sites. In Fig.2(a), we show the definitions of coordinates and primitive vectors which specifies the geometry of the ribbon. For this purpose we introduce the two vectors, $T = (m, n) = ma_1 + na_2$ and $W = (0, l) = l\mathbf{a}_2$, where $l, m, n$ are integers. The pure zigzag ribbon corresponds to $m = -n$ and the pure armchair edge is given by $m = n$.

Fig.2(b) and (c) show the energy band structures of ribbons with the general edge structures of $W = (0, 20)$ and (b) $T = (-4, 3)$ and (c) $T = (-6, 5)$ are shown. As we expected, the partially flat bands due to localized edge modes appear which break the balance between left- and right-going modes in the two valleys. Both examples are rather close to the zigzag edge so that the two valleys are well separated. In this case PCC can appear. If the geometry of
the ribbons deviates more strongly from the zigzag condition, the valley structure will become less favorable for creating a PCC, as the momentum difference between valleys shrinks. It is important to note that the extended unit cell along these generalized ribbons reduces the valley separation drastically through Brillouin zone folding. The length scale is the new effective lattice constant $a_T$ along the ribbon. Under these circumstances the condition for long-ranged impurity potentials is more stringent, $d$ being larger than $a_T$ and not $a$.

The unusual energy dispersion due to their edge states gives rise to the unique property of graphene nanoribbons. Concerning transport properties for disordered systems the most important consequence is the presence of a PCC. The origin of this effect lies in the single-valley transport which is dominated by a chiral mode. On the other hand, large momentum transfer through impurities with short-range potentials involves both valleys, destroying this effect and leading to usual Anderson localization. The obvious relation of the chiral mode with time reversal symmetry leads to the classification into the unitary and orthogonal class depending on the range of impurity potential[8]. Since the inter-valley scattering is weak in the experiments of graphene, we may assume that these conditions may be realized also for ribbons.

This work was financially supported by a Grand-in-Aid for Scientific Research from the MEXT and the JSPS (No. 19710082, No. 19310094). The numerical calculation was performed on the Grid/Cluster Computing System and HITACHI SR11000 at Hiroshima University.

References:
[1] Novoselov K S, Geim A K, Morozov S V, Jian D, Zhang Y, Dubonos S V, et. al., 2004 Science 306 666
[2] Fujita M, Wakabayashi K, Nakada K and Kusakabe K 1996 J. Phys. Soc. Japan, 65 1920
[3] Wakabayashi K, Fujita M, Ajiki H and Sigrist M 1999 Phys. Rev. B 59 8271
[4] Kobayashi Y, Fukui K, Enoki T, Kusakabe K and Kaburagi Y 2005 Phys. Rev. B 71 193406
[5] Han MY, ¨Ozyilmaz B, Zhang Y, Kim P 2007, Phys. Rev. Lett 98 206805
[6] Li X, Wang X, Zhang L, Lee S, Dai H 2008 Science 319 1229
[7] Ando T and Suzuura H 2002 J. Phys. Soc. Japan 71 2753
[8] Wakabayashi K, Takane Y, and Sigrist M 2007 Phys. Rev. Lett. 99 036601
[9] Wakabayashi K and Sigrist M 2000 Phys. Rev. Lett. 84 3390
[10] Wakabayashi K 2001 Phys. Rev. B 64 125428
[11] Ando T and Nakanishi T 1998 J. Phys. Soc. Japan 67 1704
[12] Wakabayashi K 2002 J.Phys.Soc. Japan 71 2500