

Electronic Transport Properties in Graphene Nanoribbons and Junctions

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1. Introduction

The successive fabrication of graphene devices [1,2] has initiated intensive and diverse research on carbon related systems. The honeycomb crystal structure of single layer graphene consisting of two nonequivalent sublattices conducts a unique band structure for the itinerant π -electrons near the Fermi energy, where the conduction band conically touches with the valence band, resulting in linear energy spectrum proportional to the momentum. The low-energy physical properties are formally described by “relativistic” massless Dirac equation [3], which makes strong contrast to the electronic properties of ordinary two-dimensional electron gas. In graphene, the presence of edges can have strong implications for the spectrum of the π -electrons. In graphene nanoribbons with zigzag edges, localized states appear at the edge with energies close to the Fermi level [4,5,6]. In contrast, edge states are absent for ribbons with armchair edges. Recent experiments have confirmed the existence of the edge states [7,8], and further succeeded to synthesize graphene nanoribbons using lithography techniques [9,10] and chemical techniques.[11,12,13] In this paper, we discuss the electronic properties of graphene nanoribbons and nanojunctions.

2. Electronic States of Graphene Nanoribbons

We describe the electronic states of graphene and nanoribbons by the tight-binding model. The schematic figures of graphene nanoribbons are shown in Fig.1(a) and (b). The corresponding energy band structures for sufficiently wide nanoribbons ($N=50$) are depicted in Fig.1(c) and (d). Here the parameter for energy (γ) is the transfer integral between nearest neighbor carbon sites, and is experimentally estimated about 2.75eV. In both figures, the subbands for $E<0$ ($E>0$) correspond to valence (conduction) band. The Fermi energy comes to $E=0$. The detail and pedagogical derivation for energy band structures and wavefunctions with explicit analytic form can be found in ref.[14]

The k -linear spectrum, which is signature of massless Dirac electron, appears at $k=0$ for armchair nanoribbons. Also, zigzag nanoribbons also have such linear band at $k=2\pi/3$ and $-2\pi/3$. However, the partial flat bands appears in the region of $2\pi/3 < |k| < \pi$, due to the edge states where the electrons are strongly localized near the zigzag edges. Since such edge states make a large peak in the density of states(DOS) around the Fermi energy, the existence of zigzag edges gives strong impact on the electronic properties

of graphene nanomaterials. Actually, the edge states might be responsible for unusual magnetic properties such as spin-polarized edge states[4,15], para- to dia-magnetism crossover[6], and half-metallic behaviors[16].

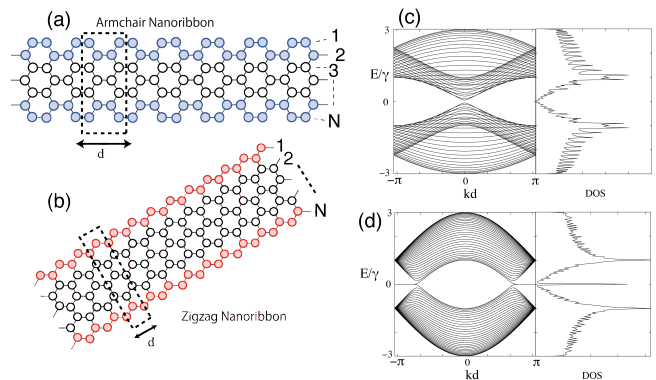


Fig 0: Schematic figures of (a) armchair and (b) zigzag nanoribbons. The rectangles with dashed lines indicate the unit cell. The energy band structure with the density of states (DOS) for (c) armchair and (d) zigzag nanoribbons ($N=50$).

3. Perfectly Conducting Channel

The presence of the partial flat bands due to edge states are not only important for magnetic properties, but also for electronic transport properties. Since graphene nanoribbons can be viewed as a new class of carbon-based quantum wires, one might expect that random impurities inevitably cause Anderson localization, i.e. conductance exponentially decays with increasing system length L and eventually vanishes. However, we can show that zigzag nanoribbons with long ranged impurities (LRI) possess a one perfectly conducting channel (PCC), i.e. the absence of Anderson localization, due to the chiral mode originating graphene edge states[17,18].

Using Landauer approach, we numerically show the presence of PCC in disordered graphene nanoribbons subjected to LRIs as shown in Fig.2(a) and (b). In clean limit ($L \rightarrow \infty$), the conductance (g) in the unit of quantum conductance ($g_0=2e^2/h$) has the following quantization rule measured from $E=0$:

$$g = 2n + 1, n=0,1,2,\dots$$

Actually we can confirm this quantization behavior in Fig.2(b) at $L=0$. The introduction of impurities (increasing L) make the decay of conductance, however, the conductance converges to 1 in the large L limit, i.e. at least one channel is perfectly conducting even in the dirty limit. The

origin of PCC is the channel imbalance induced by the existence of subband due to the edge states, where the left-going channel has one excess channel.

In armchair nanoribbons, the single-channel transport subjected to long-ranged impurities is nearly perfectly conducting, where the backward scattering matrix elements in the lowest order vanish as a manifestation of internal phase structures of the wavefunction[18,19]. However, since the intervalley scattering detrimentally dominates the electronic transport in armchair nanoribbons, such nearly perfectly conduction is available only in narrow metallic armchair nanoribbons[19,20]

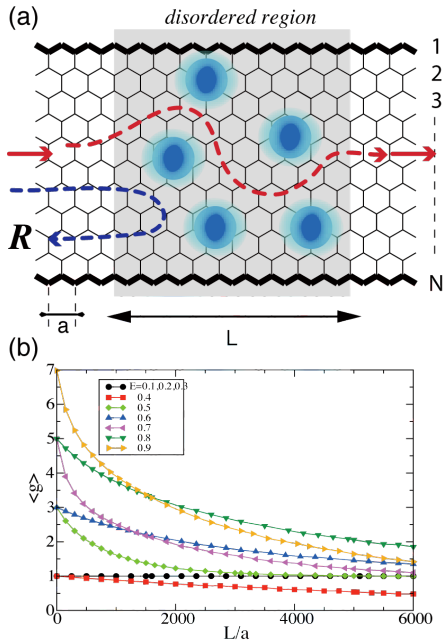


Fig 2 (a) Schematic figures of graphene nanoribbons subjected to LRIs. (b) L-dependence of averaged conductance. $\langle g \rangle$ converges to 1 in the large L limit.

3. Electronic Transport through Junctions

Since the low-energy electronic properties depend on the edge structures, the behavior of conductance can be tuned and designed by introducing the nanojunction structures[21,22]. In Fig.3, we show some typical junction structures [(a) and (b)], the (c) corresponding energy dependence of conductance and their phase of transmission coefficient[(d)]. As can be seen in Fig.3(c), the zero-conductance anti-resonances can appear depending on the junction structure. The junctions with zigzag edge have always anti-resonances in spite of that AA junction does not show such anti-resonance. Therefore, the origin of the resonances can be attributed to the coupling between zigzag edge localized states and continuum extended states, i.e. Fano resonances. This fact can be confirmed by looking at the phase of the transmission coefficient, which jumps by π at the energies that the anti-resonance occurs. Thus, tuning either the Fermi energy or local gate voltage can switch between two states, i.e., zero-conductance state ($g=0$) and nearly perfect transmission state ($g=1$).

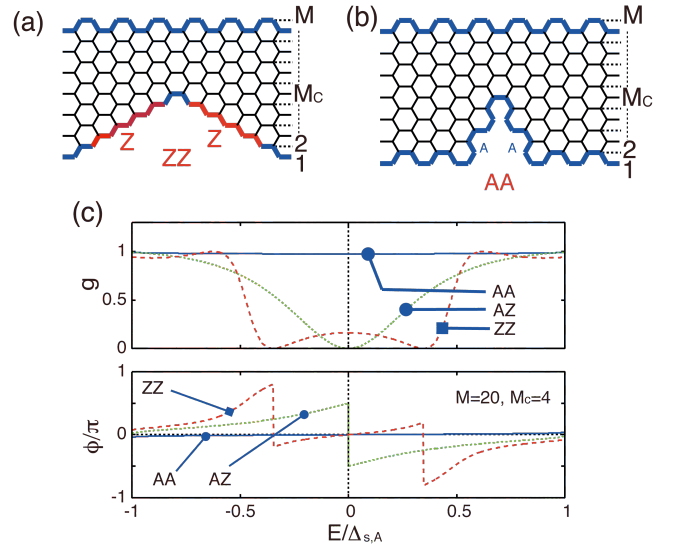


Fig 3 Schematic figures of graphene nanojunctions with (a) zigzag-zigzag (ZZ) cutting and (b) armchair-armchair cutting. (c) The Fermi energy dependence of the corresponding dimensionless conductance and phase of transmission coefficient.

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