Design of graphene waveguide: Effect of edge orientation and waveguide configuration

Nayyar Abbas Shah,1 Vahid Mosallanejad,1,∗ Kuei-Lin Chiu,2 † and Guo-ping Guo1,‡

1CAS Key Laboratory of Quantum Information, and Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Chinese Academy of Sciences, Hefei 230026, China
2Shenzhen Institute for Quantum Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China
(Dated: January 3, 2019)

Electron transport in a graphene quantum well can be analogues to photon transmission in optical fiber. In this work, we present a detailed theoretical analysis to study the possible impact of waveguide edge orientation on transport characteristics of a graphene waveguide (GW). Non-equilibrium Greens function (NEGF) approach has been utilized to investigate the transport properties of straight armchair and zigzag oriented (AO-, ZO-) GWs by considering tight-binding (TB) Hamiltonian. Plateaus at integer steps of $4e^2/h$ have been observed in both straight ZO-GW and AO-GW. Comparison of transport between these two edge orientations shows that the first quantized plateau is wider in the case of ZO-GW. Various parametric effects including the width of side-barrier, waveguide’s width and metallic property of terminals were also investigated. In addition to the observation of valley-symmetry conservation in both orientations of GWs, we have explored the critical role of the drain contact on the conductance of GWs. Furthermore, we extended our transport study to three different configurations of highly bended waveguide, such as U-shape, L-shape and split GWs, in order to explore their applications in ballistic integrated circuit devices.

I. INTRODUCTION

Combination of ballistic transport and coherent conductance quantization allows us to develop new class of nanoelectronic devices. Physically tailored graphene channel with width less than 50 nm, often noted as graphene nanoribbons (GNRs), provides an opportunity to engineer the electrical properties of the intrinsically gapless crystal. There are two different edge configurations that lead to distinct natures for GNRs; Armchair and Zigzag which are usually abbreviated as AGNR and ZGNR. Electronic properties and stability of GNRs have been investigated for realistic applications such as transistors, filters, polarizers and etc. Transport properties in these
two structures are different in many aspects, such as the spacing between conductance plateaus. Although ideal GNRs should possess the quantization of conductance, the unavoidable disorders on the edges have became dominant sources of incoherent scattering, making the quantization of conductance hardly appears in plasma-etch GNRs. Up to date, there have been few reports on the observation of quantization of conductance in GNRs which were fabricated using shadow mask and oxygen plasma etching. Further improvement is now incorporated into the design of graphene point contacts (GPC) and GNRs by applying hexagonal-born-nitride as bottom and top insulators. However, the pronounced quantization of conductance (mostly appears as kinks) is not easily accessible due to the hypersensitivity of the system to the edge disorders. On the other hand, optics-like behavior of charge carriers in graphene has revealed itself via the observation of electromagnetic phenomena such as refraction, reflections and Fabry-Pérot interference. The optics-like phenomena of electrons in graphene enables the design of all graphene electronic devices resembling an optical fiber, which effectively works as an electron waveguide. When a spatially varied electrostatic potential is imposed on graphene flakes, it can result in various devices such as graphene p-n junction, graphene tunneling junction and graphene electron waveguide (in which a uniform potential well is imposed across a graphene flake). The latter case can be regarded as the straight GWs which have been explored both theoretically and experimentally in middle and large scale geometries. In line with the previous theoretical reports (which have not been carried out by NEGF method), we have also demonstrated the quantization of conductance in straight AO-GWs and bended graphene waveguides (BGWs) by considering proper design of contacts. Since AGNR and ZGNR have very different transport properties, we aim to address a similar question: what are the distinct differences in transport between a AO-GW and a ZO-GW of similar sizes? We will divide our study into two subjects. Firstly, we present a theoretical comparison between transport in AO-GWs and ZO-GWs. Secondly, we investigate the transmission characteristics of GW with different geometries (L-shape, U-shape and split GW) in conjunction with previous studies in a small-size tailored graphene. We organize this article in the following way: the geometry of AO-GW and ZO-GW are described and the detail of our model is presented in section II. Conductance and local density of state are compared for AO-GW and ZO-GW in the first part of section III, where the quasi-one dimensional band structure for slices of AO-GW and ZO-GW are also studied for reference. The effects of geometrical parameters such as the width of side-barrier, GW and terminals were investigated. Similar transport studies were carried out for L-shape, U-shape and split GWs, and the results are presented in section IV. Conclusive remarks about all waveguide configurations will be
II. DEVICE DESCRIPTION AND METHODOLOGY

Fig. 1 illustrates the geometry of our devices. Middle-size strips of graphene with width \( W \) and length \( L \) are considered as the scattering area, where the armchair and zigzag edges are distributed along the horizontal (x-axis) and vertical directions (y-axis), respectively. We introduce an external (straight) gate to induce a spatially varied atomic on-site energy in graphene strip, which divides the scattering area into a central region of waveguide (WG) and two side-barriers (SBs). In this way, two distinct orientations for GW, i.e., AO-WG and ZO-WG, can be created as shown in Figs. 1(a) and 1(b), respectively.

\( W_G (W_{SB}) \) represents the width of waveguide (barriers) with a fixed on-site energy \( V_{WG} (V_{SB}) \) in which we have consider the full width at half maximum (FWHM) accounting for the smoothed on-site energy as shown in Fig. 1(c). The color bar represents the scale of the potential energy on the atomic sites. Each GW contains two fundamental parts, i.e. the scattering area and leads (the areas that stick out from the scattering area). We use the notation \( N_A\)-AGNR to label the central scattering area, where \( N_A \) stands for the number of dimer lines and is defined as...
\( N_A = 1 + \lfloor W/(0.5\sqrt{3}a_{cc}) \rfloor \), in which \( W \) is the width of AGNR and \( a_{cc} = 0.142 \text{ nm} \) is the carbon-carbon bond length. The length of the scattering area (L) is related with the chain number (\( N_{ch} \)) via \( N_{ch} = \lfloor L/(3a_{cc}) \rfloor \) (note that each chain contains \( 2N_A \) atoms). \( N_A \) and \( N_{ch} \) are two essential parameters to build the scattering area.

The second part of the device is contacts (source and drain) which are also made of carbon and are in fact finite-width GNRs attached to the scattering area, as illustrated by the extended GNRs sticking out of the rectangular box \( W \times L \) in Fig. 1(a) and 1(b). The width of source (drain) in AO-GW or ZO-GW is treated as an independent geometrical parameter and is labeled by \( W_S \) (\( W_D \)). The width of source (drain) is also related with the number of dimer lines in source (drain) by \( N_{eS} \) (\( N_{eD} \)), where the first index (\( e = a, z \)) stands for edge orientation. The orientation of scattering area is kept unchanged, whereas the position of semi-infinite leads and the orientation of the waveguide are different for ZO-WG and AO-WG (see Fig. 1(a) and (b)). It can be assumed that wider leads (as compare to \( W_G \)) provide denser subbands and consequently higher density of state for carriers to get in and out of the waveguide. On the other hand, wider leads may also provide extra paths for carriers to go through barriers instead of the waveguide and thus the interference may demolish the coherent transmission from source to drain. This assumption is indeed confirmed by our previous studies. Thus, in most configurations \( W_S, D \) is equal to \( W_G \) unless otherwise stated.

Moreover, our previous study has shown that a metallic AGNR is a better choice to make an ideal contact to GW\(^{38,41}\). Indeed, the zero-energy modes in a metallic AGNR permits the low energy electrons from the source to be injected into waveguide region. The advantage of using metallic GNR as leads reflects itself as an early onset of the first conductance plateau around the Dirac point. Thus, we may modify \( N_{aS, aD} \) by 1 or 2 to yield a dimer lines of \( N_A=3m+2 \), \( (m \) is an integer) which is the condition for metallic AGNR. On the other hand, ideal ZGNR leads (with even number of atoms in the unit cell) connecting to ZO-WGs do not need any modification, because naturally they have zero modes. Source leads have the same on-site energy as that in the guiding region while the drain leads are grounded (zero on-site energy) in all examples. Tight binding Hamiltonian of a graphene device can be expressed as:

\[
H = \sum_i \mu_i c_i^\dagger c_i + \sum_{i,j} t_{i,j} (c_i^\dagger c_j),
\]

where \( c_i^\dagger \) (\( c_i \)) is the creation (annihilation) operator and \( \mu_i \), indicates the on-site energy at the i-th atomic site. The on-site energy can be tuned through the external gate potentials and is in fact equal to the value of U as depicted in Fig. 1(c). Hopping between nearest neighbors (e.g., i
and \( j \) sites) is the origin of second term where \( t_{i,j} \) denotes a fixed energy value given based on TB approximation in Table I\(^{12,43}\). A small size scattering area with \( N_{ch}=3 \) is shown in Fig. 1(d) in which the 1st, 2nd and 3rd order TB approximations are indicated by blue, green and red circles, respectively. Following Landauer-Büttiker formalism, conductance of a two-terminal device in low-temperature and low-bias can be expressed as \( G = G_0 T \), where \( G_0 = 2e^2/h \) represents the quanta of conductance and \( T \) is the transmission coefficient. Spin degree of freedom is included by the factor 2 in \( G_0 \) and \( e \) and \( h \) are electron charge and the Planck’s constant\(^{44}\). Transmission coefficient from source to drain, \( T \), can be calculated using Caroli’s formula\(^{45}\):

\[
T = \text{trace}(\Gamma_s G^r \Gamma_d G^a)
\]

where \( \Gamma_s (\Gamma_d) \) is the broadening matrix of the source (drain) lead. \( G^r (G^a = G^r \dagger) \) represents retarded (advance) Greens function given by

\[
G^r(E) = [(E + i\eta)S - H - \Sigma_s(E) - \Sigma_d(E)]^{-1}
\]

where \( \eta \) is small infinitesimal number usually about \( 10^{-4} \). Here, \( S \) is the overlap matrix built in similar way to the second term in Hamiltonian and has the following form

\[
S = \sum_{i,j} s_{i,j}(c_i^\dagger c_j)
\]

where \( s_{i,j} \) represent the overlap integral between the atomic orbitals (\( p_z \)) located at \( i \) and \( j \). It is worth noting that orbitals at two different atomic sites are not necessarily orthogonal to each other. Therefore, there are non-zero values in the \( S \) matrix considering 3rd third nearest approximation but these values are small due to long distance interactions between atomic orbitals. Open boundary condition at the source and drain is incorporated into the transport study via the last two terms in equation (3), which are the so called self-energy terms. Self-energy matrices are calculated via

\[
\Sigma_s = A_s^\dagger g_s A_s \quad \text{and} \quad \Sigma_d = A_d^\dagger g_d A_d,
\]

in which \( A_s, d \) are given by

\[
A_{s, d}(E) = [(E + i\eta)S_s, s_d - H_s S, s_d]
\]

| approx. | \( \epsilon_0(eV) \) | \( t_0(eV) \) | \( t_1(eV) \) | \( t_2(eV) \) | \( s_0(eV) \) | \( s_1(eV) \) | \( s_2(eV) \) |
|---------|----------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 1st\(^{22}\) | 0 | -2.74 | 0 | 0 | 0 | 0 | 0 |
| 3rd\(^{43}\) | -0.36 | -2.78 | -0.12 | -0.068 | 0.106 | 0.001 | 0.003 |

TABLE I: Hopping energies and overlap integral values for 1st (at the first row) and 3rd (at the second row) nearest neighbor TB approximation.
Here, $H_{sS}$ and $S_{sS}$ are the *Interaction Hamiltonian* and *Interaction overlap* matrices between the source and the first super cell in the scattering area, while $H_{Sd}$ and $S_{Sd}$ are the *Interaction Hamiltonian* and *Interaction overlap* matrices between the last supercell in the scattering area and drain lead (index $S$ refers to the scattering area whereas $s$ and $d$ denote the source and drain).

In process of building $H_{sS}$ ($S_{sS}$), the $i$ index from equation (1) (and equation (4)) goes over atomic sites in the source lead while the $j$ index goes over sites in the first super-cells of central scattering area. $H_{Sd}$ and $S_{Sd}$ are constructed similarly. Sancho-Rubio iterative scheme is employed to calculate the retarded surface Greens functions, $g_{s,d}$. One can easily obtain *broadening matrices* as $\Gamma_{s,d} = i(\Sigma_{s,d} - \Sigma_{s,d}^\dagger)$. Another important parameter is the local density of state (LDOS) given by

$$\text{LDOS}(E) = \left(\frac{i}{\pi}\right)\text{diag}(G^r(E) - G^a(E))$$ (6)

where *diag* refers to the diagonal elements of the matrix. LDOS can also be evaluated by extracting the real part of the diagonal elements of spectral function $(G^r\Gamma_{s,d}G^a)$. This parameter basically determines the spatial distribution of wave function in certain Fermi energy. Inversion of the large matrix in equation (3), associated with the large number of atoms in scattering area, is a massive task for a computation machine. For many of the physical quantities such as transmission function and LDOS, only parts of the full Green’s function are required. The recursive scheme, explained in details in Ref.47, aids us to obtain the essential parts of the Greens function. In tight-binding theory, expansion of free electron wave function in terms of the Block’s wavefunction together with the minimization of energy converts the Schrödinger equation into an eigenvalue matrix equation, $H(k) - E(k)S(k) = 0$, where $k$ is the two dimensional wavevector whose range is determined by high symmetry points in graphene’s reciprocal lattice. In systems with a physical confinement in the transverse direction, it is possible to further simplify the 2D bandstructure calculation by assuming a plane-wave wavefunction in the longitudinal direction i.e., $e^{ik_\|x\|}$ where the index $\|$ denotes the transport direction. Physical confinement in transverse direction leads to $H(k_\perp) - E(k_\perp)S(k_\perp) = 0$.

The eigenvalues $E(k_\perp)$ of the characteristic equation, which is the so-called *secular equation*, is written as

$$\det(H(k_\perp) - E(k_\perp)S(k_\perp)) = 0,$$ (7)

gives the quasi-one dimensional bandstructure. Note that $H(k_\perp)$ is defined by

$$H(k_\perp) \equiv H_{ke}e^{-i k_\perp a_c} + H_{cc} + H_{cr}e^{i k_\perp a_c}$$ (8)
where $a_c$ is the distance between the neighbor super-cells, and $H_{lc}$, $H_{cc}$ and $H_{cr}$ represent the TB interaction Hamiltonian (TB-IH) between atoms in the left and central super-cells, TB-IH between atoms in central super-cell, and TB-IH between atoms in central super-cell and the right super-cell, respectively. One must use equation (1) to build each of these three Hamiltonian matrices. $S(k_\perp)$ has similar form as $H(k_\perp)$ in which $S_{lc}$, $S_{cc}$ and $S_{cr}$ (constructed via equation (4)) are now replacing the equivalent Hamiltonian terms in equation (8).

III. RESULTS AND DISCUSSIONS

A. A. Straight Waveguides

In our devices, two types of edge orientations (AO-GWs, ZO-GWs) for straight GW are studied for three devices with different side-barrier’s width ($W_{SB}$) to investigate the effect of $W_{SB}$ on transport. The length ($L$) and the width of the guiding region ($W_G$) are fixed at 100 nm and 20 nm, respectively. The latter is equivalent to $NA-GW=163$ for AO-GW and $NZ-GW=188$ for ZO-GW, and the total width $W$ is 40, 60 and 80 nm which corresponds to $W_{SB}=10$, 20 and 30 nm. At the same time the dimer number of leads $N_{aS}, aD=161$ (metallic armchair leads) and $N_{zS}, zD=188$ (symmetric zigzag leads) have been considered for AO-GW and ZO-GW, respectively. Transport studies have been carried out for these six samples by considering both first (1NN) and third (3NN) nearest TB approximations and the results are shown separately on the left and right panels in Fig. 2.

On-site potential energy in scattering area is smoothly varied within $\Delta W=44a_{cc} \approx 6.25$ nm from $V_{SB}=0$ eV at the side-barriers to $V_{WG}=-0.3$ eV at the guiding area for all twelve devices. As mentioned earlier, the source leads are considered at the same potential as in waveguide area ($V_{WG}$) but drain leads are grounded in all samples. In Fig. 2 both the 20nm ZO-WG and AO-WG exhibit a quantization of conductance, with a value of $G=1, 3, 5 G_0$ in the same configurations(with the same $W_{SB}$). The first plateau of ZO-WG is clearly wider in energy axis than that of AO-WG. The first plateaus of conductances of both ZO-WG and AO-WG are flat whereas other higher plateaus are not exactly flat and gradually lose their flatness toward positive energies. Importantly, the effect of SB (different $W_{SB}$) seems negligible for both orientations, which suggests the minimum influence of edge disorders in a possible GW as long as the edges (the border between side-barrier and vacuum) are far enough (e.g. half of $W_G$) from the waveguide area.

When 3NN Hamiltonian is employed, other differences in conductance became visible: e.g.
FIG. 2: Conductance of 20 nm-wide AO-WG (red-dot lines) and ZO-WG (green-solid lines) with varying the side-barrier width, $W_{SB}$. (a)-(c) with 1NN approximation and (d)-(f) with the 3NN approximation.

FIG. 3: Conductance of source (blue-dot line), drain (red-dashed-dot line) and ZO-GW (green-solid line) considering (a) 1NN and (b) 3NN.

conductance for ZO-WG exhibits higher values on $E<0$ eV. This difference can be explained by comparing the conductance of the drain electrode and AO-GW under the third nearest neighbor approximation, as shown in Fig. 3. Note that, conductances of the drain electrode refers to the conductance of the semi-infinite nanoribbon on the drain lead. The correspondence between the red-dashed-dot line and green-solid line in Fig. 3 suggests that the conductance of our system follows the conductance behavior of the drain terminal. With 3NN approximation, noticeable dips in conductances around $E=0$ eV for AO-WGs (red-dot lines) have appeared at Figs. 2(d)-(f), which can be understood by the fact that 3NN tends to yield a small band gap in an AGNR (i.e. terminals). Both 1NN and 3NN give rise to noisy conductance features at $E<0$ eV in ZO-GW.
FIG. 4: (Color online) The effect of leads size on transport of GWs considering $W_{SB}=20$ nm and $W_{G}=20$ nm. On the first row (a) and (b) show conductances for different combination of metallic/nonmetallic (m/n) leads on AO-GW and ZO-GW respectively. On the second row, (c) and (d) shows conductances for various widths of metallic leads on AO-GW and ZO-GW.

Similar noisy conductance has also been observed in AO-GW but in much lower energies e.g. $E<0.2$ eV (not shown in Figs. 2). We attribute these noises to the increase of current going through side barriers in this range of energy. Plateaus gradually disappear at higher energies because there are limited confined wavefunctions belong to the waveguide area.

We further explore the effect of lead on GWs transport properties. Here, we modified the dimer lines of leads by 1 or 2 to make leads either metallic or semiconducting (nonmetallic). In contrast to the insensitivity of conductance to the widths of side-barriers, conductances for both orientations show clear sensitivity to metallic/nonmetallic (m/n) nature of leads, as shown in Fig. 4(a) and 4(b). One third of AGNRs and an ideal ZGNR have metallic behavior because their band structures possess zero mode. Different combinations of metallic and non-metallic leads are considered for a previously studied configuration, $W_{SB}=20$ nm and $W_{G}=20$ nm. Non-metallic drain on AO-GW yields a finite gap on conductance around $E=0$ eV (orange-solid and green-dot lines in Fig. 4(a)) while the conductance of a configuration with solely non-metallic source is identical to that with both metallic leads (blue-solid line is identical to red-dot line in Fig. 4(a)). Moreover, the conductance of AO-GW with non-metallic drain (m-n and n-n), shows shorter plateaus with quantization steps of $G_0$ compared to that with metallic drain (n-m and m-m).
Note that an ideal zigzag lead (with closed hexagonal crystal structure) represented by an even dimer lines is indeed metallic, however, odd number of dimer lines for ZGNRs results in breaking the crystal symmetry and thus its dispersion relation no longer possess the zero-mode energy. Gap on conductance is even wider in the case of ZO-GW with disordered (non-metallic) drain (green-dot line in Fig. 4(b)). Here, we refer a ZGNR lead with odd number dimer lines as a disordered lead. Also, like AO-GW, the conductance of ZO-GW with non-metallic source and metallic drain (n-m) is identical to that with both metallic leads (m-m), as shown by the blue-solid and red-dot lines in Fig. 4(b). Non-metallic drain (m-n and n-n) on ZO-GW does not change the quantization step (in contrast to AO-GW) but it has shifted the conductance both vertically and horizontally, as shown in Fig. 4(b). This result again indicates that the nature of drain plays a significant role on the conductance for GW with both orientations. Therefore, we adopted metallic leads for the rest of our studies because they yield early onset of plateau on conductance for both edge orientations. Varying lead width at nanometer scale also influences the conduction of GW for both edge orientations, as shown in Fig. 4(c) and 4(d). Wider conductance plateaus are presented for short leads and vice versa. The situation \( W_{D,S} \neq W_G \) has added a visible level of noise to the conductance plateaus in much shorter (16 nm) and much wider (40 nm) leads as compared to the primary case of \( W_{D,S} = W_G \).

Afterwards, the effect of parameter \( W_G \) on conductance of GW is compared between both edge orientations. We consider three values of \( W_G = 20, 30 \) and 40 nm (and making \( W_{D,S} = W_G \)) while length \( L = 100 \) nm and side-barriers \( W_{SB} = 20 \) nm are kept fixed. Conductances and quasi-one dimensional band structures of supercells corresponding to each \( W_G \) are plotted in Fig. 5 with the same color schemes. For both edge orientations, as \( W_G \) decreases from 40 nm to 20 nm, conductance plateaus get longer as a result of larger spacing between the energy bands, as visible in Fig. 5(b)-(d) and (f)-(h). Note that subbands of AO-GW (see Fig. 5(b)-(d)) are two-fold degenerate while subbands of ZO-GW (see Fig. 5(f)-(h)) are not degenerate. One can deduce that the first plateau on conductance for \( E > 0 \) eV has not been originated from the first band of GW by tracking the background gray dashed lines between the conductance and bandstructure in Fig. 5. For instance, the forth band of 20 nm wide GW in Fig. 5(d) (bands are named by numbers regardless of degeneracy) around \( E = 0 \) eV coincides with the beginning of the first plateau in Fig. 5(a) (solid-green line). To further explore the transport properties of GW in two different edge orientations, local density of states (LDOS) are calculated for the case of \( W_G = 20 \) nm. In Figs. 6(a)-6(d), normalized LDOS for both AO-GW and ZO-WG are presented at two Fermi energies, \( E_1 = 0.05 \) eV and \( E_2 = 0.15 \) eV, which correspond to the conductances of \( G_0 \) and \( 3G_0 \), respectively. Right panels
FIG. 5: (Color online) (a) Conductances of AO-GWs for various $W_G=20, 30$ and 40 nm. (b)-(d) band structure plots for different $W_G$ on (a). (e) Conductances of ZO-GWs for various $W_G$ similar to (a). (f)-(h) band structure plots for corresponding $W_G$ of (e).

of Figs. 6(a)-6(b) and lower panels of Figs. 6(c)-6(d) show the average of unnormalized LDOS ($<\text{LDOS}>$) within the black-dashed lines. Reasonable localization of LDOS is present within the waveguide area at $E_1$ for both AO-GW and ZO-WG, as shown in Figs. 6(a) and 6(c). The four peaks visible on the $<\text{LDOS}>$ (right panel) in Fig. 6(a) correspond to the fourth mode in the band structure of AO-GW (see Fig. 5(d)), which contributes to the first plateau for $W_G=20$ nm. Similar analysis can be performed for other GW with different widths and at different energies. Comparison between Fig. 6(a) and Fig. 6(b) (or Figs. 6(c) and Fig. 6(d)) shows stronger confinement of wavefunction at $E_1$ as compare to $E_2$. Nevertheless, $<\text{LDOS}>$ show that leakages toward side barriers for both edge orientations are still neglectable at $E_2$.

B. B. U-, L-Shape and Split Waveguides

Two other types of two-terminal curved waveguides, U-shape and L-shape, have been taken into account to investigate the electronic transport and the abilities to confine the charge particles in these highly bended geometries. In a U-shape graphene waveguide (U-GW), both source and drain leads are connected to the same edge orientation (either all AO or all ZO). A U-AO-GW (U-ZO-GW) can be constructed when a straight AO-GW (ZO-GW) bends 180° as shown in
FIG. 6: (Color online) LDOS for AO-WG (a) at $E_1=0.05$ eV and (b) at $E_2=0.15$ eV. Right panels on (a) and (b) show the average of unnormalized LDOS between selected region by black-dashed lines. (c) and (d) show the LDOSs and average of unnormalized LDOSs at $E_1$ and $E_2$ of ZO-GW.

Device dimensions of $W \times L=120$ nm $\times 80$ nm are considered for U-AO-GW and $W \times L=80$ nm $\times 120$ nm for U-ZO-GW. The width of middle barrier between source and drain ($=2R_1$, see Fig. 7(a) and 7(b)) is set to 40 nm (30 nm) when $W_G=20$ nm (30 nm), while $W_{SB}=20$ nm has been used for both U-AO-GW and U-ZO-GW. In the case of U-AO-GW with $W_G=20$ nm, the on-site energy of device is constructed by a combination of three segments: two parts of AO-GW with $L=20$ nm which are parallel to each other, and half of a circular waveguide loop with inner (outer) radius of 20 nm (40 nm) that provides a smooth 180° bending around the center of the circular part ($x_c=20$ nm, $y_c=60$ nm, see Fig. 7(a)). U-ZO-GW is also constructed similarly, see Fig. 7(b). Conductance of U-AO-GWs and U-ZO-GWs both resemble the conductance of their counterparts AO-GWs and ZO-GWs (compare Fig. 7(c) with Fig. 5(a) for $W_G=20$ nm and com-
FIG. 7: (Color online) (a) and (b) show schematic diagram of U-AO-GW and U-ZO-GW. (c) and (d) shows the conductances of U-AO-GW and U-ZO-GW respectively with $W_G=20$ nm (red-dot line), 30 nm (green-solid line). LDOS of $W_G=20$ nm U-GWs are presented in (e) and (f) for $E=0.03$ eV.

pare Fig. 7(d) with Fig. 5(e) for $W_G=20$ nm). In the U-shape case, the general form of quantized conductance is preserved but the second plateau is modulated by a visible oscillation as highlighted by a dashed ellipse in Fig. 7(d). This oscillation is more pronounced for the $W_G=20$ nm case and it becomes weaken when $W_G=30$ nm. Considering $W_G=20$ nm, normalized LDOSs for U-AO-GW and U-ZO-GW at a given energy of $E=0.03$ eV (which locates within the first plateau) are plotted in Figs. 7(e) and (f), respectively. Both LDOS show reasonable confinement at the given energy.

Next, we consider the L-shape graphene waveguide (L-GW) to investigate the effect of 90° bending on GW’s transport properties. In a L-shape GW, source and drain are not attached to the same edge orientation in the scattering area. Two possible configurations are included: I) L-GW with an AO-GW bending to a ZO-GW (with source on zigzag interface and drain attached to the armchair interface), labeled as L-AZ-GW; II) L-GW with a ZO-GW bending to a AO-GW (here the source is on armchair interface and drain is on zigzag interface), labeled as L-ZA-GW. In both cases, we
have considered \( W = L = 100 \text{ nm} \) for the scattering area and the waveguide (hence the on-site energy) is constructed by the combination of three parts: a AO-GW and a ZO-GW (both with \( L = 50 \text{ nm} \)) perpendicular to each other, and a quarter of a circular waveguide with inner (outer) radius of 10 nm (30 nm) which provides a smooth 90° bending around the center of the system \((x_c = 50 \text{ nm}, \ y_c = 50 \text{ nm}, \ \text{see Figs. } 8\text{(a) and } 8\text{(b)})\). To calculate the conductance of the aforementioned configurations, one only needs to switch the on-site energies between source and drain and also the relative positions of \( \Gamma_s \) and \( \Gamma_d \) in Eq. 2. Conductance of L-AZ-GW and L-ZA-GW, each with two values of \( W_G = 20 \text{ nm} \) and 30 nm, are plotted in Figs. 8(c) and 8(d), respectively. Consistent with the previous GW conductance of L-GWs for ZA and AZ both show dependence on the nature of the drain (compare Fig. 8(c) with Fig. 5(a) and compare Fig. 8(d) with Fig. 5(e) for both \( W_G = 20 \text{ nm} \) and 30 nm). Conductance of a 20 nm L-ZA-GW also possess a visible oscillation at the second conductance plateau, similar to the case of U-WGs. This phenomenon might be attributed to the bending induced scattering between \( K \) and \( K' \) sub lattices. Similarly, we calculated the LDOS of L-GWs with \( W_G = 20 \text{ nm} \) and at \( E = 0.05 \text{ eV} \) (in the first conductance plateau). Both L-GWs present visible confinement of wave function along the straight parts and around the bending area, as observed in Figs. 8(e) and 8(f).

As an extension to L-GW, the split waveguides (SP-GWs), which can be viewed as the counterpart of an optical beam splitter, has been studied. On-site energy of a SP-GW can be set-up by adding the on-site energy of two adjacent L-GWs which are bended in opposite directions. SP-GWs can be divided into two parts, i.e. the stem part and two split parts, within the scattering area. In our example, the width of stem part is \( W_G = 40 \text{ nm} \) and it splits equally into two 20 nm wide bended WGs. We also considered two categories for SP-GWs which are labeled by the orientation of the stem part and the branches part (i.e., AZ (ZA), which mean A (Z) for stem and Z (A) for branches). Drains at the end of branches are connected to different interfaces, which are opposite to the stem, due to the 90° bending of each L-shape waveguides. In Figs. 9(a) and 9(b), conductance is labeled by numbers. The first number, 1, indicates the stem while the second, 2 or 3, refers to each branches. Conductance for both paths in the three-terminal SP-AZ-GW show similar trend to that of 20 nm ZO-GW. The conductance of SP-ZA-GW also follows a similar behavior of the 20 nm AO-GW, which can be recognized by a small dip on conductance around \( E = 0 \text{ eV} \) (see Fig. 9(b)). Thus, it can be concluded that the same role of drain nature (the type of drain interface and drain width) on conductance is also applicable for the split structures.

These results are also consistent with our previous work where the source and drain of the Y junction graphene waveguide are attached to the same type of interfaces. Again, we plot the
FIG. 8: (Color online) Schematic diagram of (a) L-AZ-GW and (b) L-ZA-GW. (c) and (d) show the conductances of L-AZ-GW and L-ZA-GW, with $W_G=20$ nm (red-dot line) and 30 nm (green-solid line), respectively. LDOS of $W_G=20$ nm L-GWs are presented on (e) and (f) at $E=0.05$ eV.

normalized LDOS of split waveguides in Figs. 9(c) and 9(d) to depict the effect of confinement at $E=0.05$ eV for each category. In addition, quasi-one dimensional band structures for selected supercells around the splitting point, indicated by dashed rectangle in Figs. 9(c) and 9(d), are plotted in Figs. 10(a) and 10(b), respectively.

We have chosen these segments of the scattering area, because they can give us the energy bands right at the beginning of two independent branches. Moreover, it was shown that guiding energy bands are not highly sensitive to bending.

Energy bands show the two-fold (Fig. 10(b)) and four-fold (Fig. 10(a)) degeneracy for supercells with zigzag (Fig. 9(c)) and armchair (Fig. 9(d)) edges which comparing to the straight GWs (see Figs. 5(b)-(d) and Figs. 5(f)-(h)) the number of energy bands in the presence of branches has doubled. Each of two-fold energy bands in Fig. 10(b) can be refers to a nondegenerate energy band of each branches. Similarly, One can divide four-fold degenerate energy bands in Fig. 10(a)
FIG. 9: (Color online) (a) and (b) show conductances of SP-ZA-GW and SP-AZ-GW with $W_G=40$ nm for stem and $W_G=20$ nm for branches. LDOS of SP-ZA-GW and SP-AZ-GW are presented in (c) and (d) at $E=0.05$ eV.

into two two-fold degenerate bands of each branches. Moreover, the symmetry of system along the transport direction (the stem part) assure the spatial continuity of energy channels along each branch segments. Therefore, incoming wave has equal probability to scatter into each branches at the splitting point and result in ballistic transport from splitting point to drains. This justifies the similarity in conductance between each branch (see Figs. 9(a) and 9(b)).

IV. CONCLUSION:

In this article, we first present a comparative transport study between two types of straight graphene waveguides with different edge orientations, i.e. armchair and zigzag. Differences and similarities in transport have been studied between them by performing series of analyses on conductance features. We concluded that the conductance in both armchair and zigzag oriented waveguides can be quantized by steps of $(4e^2/h)$ in a similar manner, but the zigzag oriented waveguide shows a longer first plateau provided that its drain terminal possesses zero energy mode. Moreover, the effect of TB approximation, width of side barrier, width of waveguide and terminal geometry on the conductance have all been included in our investigation. Our results indicated that the conductance of a graphene waveguide primarily follows the conductance property of the drain terminal regardless of the orientation and degree of bending of the main GW.
FIG. 10: Band structure of branch waveguides around splitting area for zigzag (a) and armchair (b) edge nanoribbons. Where green, red, solid and dotted lines are distinguishing degenerated sub-bands.

LDOS maps for all configurations at different Fermi energies have been extracted, which show that highly bended waveguides are also very capable of confining charge particles at energies around the first conductance plateau. Altogether, our studies clarify the nature of quantum transport in graphene waveguide with realistic terminals and thus are useful for the application of graphene in modern nanoelectronic devices. Robust conductance quantization on highly bended GWs makes them a possible replacement to conventionally used metallic wires, and thus making all-graphene integrated circuits possible in the future.

V. ACKNOWLEDGMENTS

This work was financially supported by the National Key Research and Development Program (Grant No. 2016YFA0301700), NNSFC (Grant Nos. 11625419 and 11474265), and the China Government Youth 1000-Plan Talent Program. The Supercomputing Center of USTC is gratefully acknowledged for high-performance computing assistance. This was also supported by Chinese Academy of Sciences and The World Academy of Science for the advancement of science in devel-
oping countries.

Correspondence author: vahid@ustc.edu.cn
Correspondence author: eins0728@gmail.com
Correspondence author: gpguo@ustc.edu.cn

1 B. Van Wees, H. Van Houten, C. Beenakker, J. G. Williamson, L. Kouwenhoven, D. Van der Marel, and C. Foxon, Physical Review Letters 60, 848 (1988).
2 D. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J. Frost, D. Hasko, D. Peacock, D. Ritchie, and G. Jones, Journal of Physics C: solid state physics 21, L209 (1988).
3 S. Somanchi, B. Terrés, J. Peiro, M. Staggenborg, K. Watanabe, T. Taniguchi, B. Beschoten, and C. Stampfer, Annalen der Physik 529, 1700082 (2017).
4 F. Akbar, M. Kolahdouz, S. Larimian, B. Radfar, and H. Radamson, Journal of Materials Science: Materials in Electronics 26, 4347 (2015).
5 M. Connolly, K. Chiu, S. Giblin, M. Kataoka, J. Fletcher, C. Chua, J. Griffiths, G. Jones, V. Fal’Ko, C. Smith, et al., Nature nanotechnology 8, 417 (2013).
6 M.-L. Zhang, D. Wei, G.-W. Deng, S.-X. Li, H.-O. Li, G. Cao, T. Tu, M. Xiao, G.-C. Guo, H.-W. Jiang, et al., Applied Physics Letters 105, 073510 (2014).
7 M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, Journal of the Physical Society of Japan 65, 1920 (1996).
8 Y.-W. Son, M. L. Cohen, and S. G. Louie, Physical review letters 97, 216803 (2006).
9 M. Y. Han, B. Özyilmaz, Y. Zhang, and P. Kim, Physical review letters 98, 206805 (2007).
10 Y. Hancock, A. Uppstu, K. Saloriutta, A. Harju, and M. J. Puska, Physical Review B 81, 245402 (2010).
11 V. Barone, O. Hod, and G. E. Scuseria, Nano letters 6, 2748 (2006).
12 F. Schwierz, Nature nanotechnology 5, 487 (2010).
13 P. Ruffieux, J. Cai, N. C. Plumb, L. Patthey, D. Prezzi, A. Ferretti, E. Molinari, X. Feng, K. Mullen, C. A. Pignedoli, et al., Acs Nano 6, 6930 (2012).
14 Q. Bao, H. Zhang, B. Wang, Z. Ni, C. H. Y. X. Lim, Y. Wang, D. Y. Tang, and K. P. Loh, Nature photonics 5, 411 (2011).
15 Z. Zhu, C. Guo, K. Liu, J. Zhang, W. Ye, X. Yuan, and S. Qin, Journal of Applied Physics 116, 104304 (2014).
16 T. Li and S.-P. Lu, Physical Review B 77, 085408 (2008).
17 M. Evaldsson, I. V. Zozoulenko, H. Xu, and T. Heinzel, Physical Review B 78, 161407 (2008).
18 N. Djavid, K. Khaliji, S. M. Tabatabaei, and M. Pourfath, IEEE Transactions on Electron Devices 61, 23 (2014).
19 M. Y. Han, J. C. Brant, and P. Kim, Physical review letters 104, 056801 (2010).
20 C. Lian, K. Tahy, T. Fang, G. Li, H. G. Xing, and D. Jena, Applied Physics Letters 96, 103109 (2010).
21 Y.-M. Lin, V. Perebeinos, Z. Chen, and P. Avouris, Physical Review B 78, 161409 (2008).
22 A. S. M. Goossens, S. C. Diressen, T. A. Baart, K. Watanabe, T. Taniguchi, and L. M. Vandersypen, Nano letters 12, 4656 (2012).
23 B. Terrés, L. Chizhova, F. Libisch, J. Peiro, D. Jörger, S. Engels, A. Girschik, K. Watanabe, T. Taniguchi, S. Rotkin, et al., Nature communications 7, 11528 (2016).
24 H. Overweg, H. Eggimann, X. Chen, S. Slizovskiy, M. Eich, R. Pisoni, Y. Lee, P. Rickhaus, K. Watanabe, T. Taniguchi, et al., Nano letters 18, 553 (2017).
25 N. Tombros, A. Veligura, J. Junesch, M. H. Guimarães, I. J. Vera-Marun, H. T. Jonkman, and B. J. Van Wees, Nature Physics 7, 697 (2011).
26 V. Clericò, J. A. Delgado-Notario, M. Saiz-Bretín, C. Hernández Fuentevilla, A. V. Malyshev, J. D. Lejarreta, E. Diez, and F. Domínguez-Adame, physica status solidi (a) p. 1701065 (2018).
27 P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönemberger, Nature communications 4, 2342 (2013).
28 S. Chen, Z. Han, M. M. Elahi, K. M. Habib, L. Wang, B. Wen, Y. Gao, T. Taniguchi, K. Watanabe, J. Hone, et al., Science 353, 1522 (2016).
29 V. V. Cheianov, V. Fal’ko, and B. Altshuler, Science 315, 1252 (2007).
30 T. Low and J. Appenzeller, Physical Review B 80, 155406 (2009).
31 Z. Wu, Applied Physics Letters 98, 082117 (2011).
32 R. R. Hartmann, N. Robinson, and M. Portnoi, Physical Review B 81, 245431 (2010).
33 J. Williams, T. Low, M. Lundstrom, and C. Marcus, Nature Nanotechnology 6, 222 (2011).
34 P. Rickhaus, M.-H. Liu, P. Makk, R. Maurand, S. Hess, S. Zihlmann, M. Weiss, K. Richter, and C. Schonenberger, Nano letters 15, 5819 (2015).
35 Y. He, M. Ding, Y. Yang, and H. Zhang, Superlattices and Microstructures 85, 761 (2015).
36 M. Kim, J.-H. Choi, S.-H. Lee, K. Watanabe, T. Taniguchi, S.-H. Jhi, and H.-J. Lee, Nature Physics 12, 1022 (2016).
37 S.-M. Cao, J.-J. Zhou, X. Wei, and S.-G. Cheng, Journal of Physics: Condensed Matter 29, 145301 (2017).
38 V. Mosallanejad, K. Wang, Z. Qiao, and G. Guo, Journal of Physics: Condensed Matter 30, 325301 (2018).
39 Y. E. Xie, Y. P. Chen, L. Sun, K. Zhang, and J. Zhong, Physica B: Condensed Matter 404, 1771 (2009).
40 C. G. da Rocha, R. Tuovinen, R. van Leeuwen, and P. Koskinen, Nanoscale 7, 8627 (2015).
41 V. Mosallanejad, K.-L. Chiu, and G.-P. Guo, Journal of Physics: Condensed Matter 30, 445301 (2018), URL http://stacks.iop.org/0953-8984/30/i=44/a=445301.
42 S. Reich, J. Maultzsch, C. Thomsen, and P. Ordejon, Physical Review B 66, 035412 (2002).
43 R. Kundu, Modern Physics Letters B 25, 163 (2011).
44 S. Datta, Quantum transport: atom to transistor (Cambridge university press, 2005).
45 C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, Journal of Physics C: Solid State Physics 4, 916 (1971).
46 M. L. Sancho, J. L. Sancho, J. L. Sancho, and J. Rubio, Journal of Physics F: Metal Physics 15, 851 (1985).
47 G. Thorgilsson, G. Viktorsson, and S. Erlingsson, Journal of Computational Physics 261, 256 (2014).
48 R. Saito, G. Dresselhaus, and M. S. Dresselhaus, Physical properties of carbon nanotubes (World Scientific, 1998).
49 W.-X. Wang, M. Zhou, X. Li, S.-Y. Li, X. Wu, W. Duan, and L. He, Physical Review B 93, 241403 (2016).