Perfectly conducting graphene electronic waveguide with curved channels

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Abstract

We theoretically investigate the electronic transport properties of curved graphene waveguides by employing non-equilibrium Green’s function techniques. We systematically study the dependence of the confined waveguide modes on the potential difference, the width of waveguide and side barrier. Through two-terminal electronic transport calculations, we show that the conductance of confined waveguide modes is rather robust against the bending degree of waveguide, in consistence with the band insensitivity to the side barrier. This finding of the perfectly conducting channels strongly suggests the possibility of applying the graphene waveguide in the design of low-power nanoelectronics.

Keywords: electronic transport, graphene, electronic waveguide

(Some figures may appear in colour only in the online journal)

1. Introduction

Due to its linear Dirac dispersion, graphene exhibits excellent physical properties, including the electronic and optical aspects \cite{1–3}. All these made graphene a promising candidate for designing future electronics. However, the intrinsic zero-gap of graphene hindered the possibility of replacing silicon to realize the basic on/off function of semiconductors. Subsequent efforts have been made to explore various two-dimensional (2D) materials that naturally harbour bulk band gaps, e.g. silicene \cite{4} and transition metal dichalcogenide MX\textsubscript{2} \cite{5}. Although a variety of new 2D materials become constantly proposed in theory and discovered in the experiment, high mobility of graphene at room temperature \cite{6} has attracted overwhelming attention. Both theoretical and experimental researchers continue exploiting graphene-based electronics via external manipulation after a dozen years ever since its first experimental discovery.

Two-component wavefunction in graphene, so-called pseudospin, results in extraordinary tunneling phenomena, namely Klein tunneling \cite{7}. This phenomenon is in close conjunction with suppression of backscattering in graphene and responsible for the high mobility in the single-layer graphene lattice. In the presence of uniform potential well i.e. confined regime, however, the equation of motion can be reduced to an Eigen-value equation that resembles the Helmholtz equation in optics \cite{8}. In particular, optic-like phenomena such as Goos–Hanchen and Veselago lens effects, have been studied in graphene \cite{9–11}. Extensive theoretical calculations have been carried out to investigate electronic modes in graphene waveguide by solving Dirac–Weyl equation \cite{12–18}. As a result, the separation of several waveguide modes from the other conic subbands (corresponding to barriers modes) and sporadic conversion of valance subbands to the conduction subbands, are observed. It has commonly been assumed that the transport through graphene waveguide can be classified...
into two regimes: (1) The optical waveguide regime, often called total reflection regime, which can occur when the barriers and waveguide have the same polarity; (2) p-n guiding regime, where the polarity of carriers between barriers and waveguide are different [19, 20]. Confinement of carriers in a n-p-n junction is demonstrated in latest experimental studies [21, 22]. Furthermore, kinked graphene waveguide based on graphene antidot has been proposed [23]. Exotic phenomena, such as snake states, have been realized in graphene p-n junction [24–26]. Most interestingly, recent experimental and theoretical studies have shown the valley-degenerate transport in graphene waveguide with arbitrary chiral orientation, except armchair edge [27, 29].

Theoretically, graphene waveguide [19, 29] can be achieved by externally applying a hard-wall square-shape potential well in the transverse direction (see figure 1(a)). This should be experimentally feasible with recent advances in the fabrication techniques and applying thin film insulators (e.g. hexagonal boron nitride). So far, both theoretical and experimental studies have been mainly concentrated on the straight graphene waveguides. Moreover, the ballistic transport of the confined states in the quantum well has been experimentally demonstrated [19, 20]. It is well-known that one of the most striking features of optical fibers is that the electromagnetic waves can efficiently transmit in any kinds of bending. This is directly applied in the field of information communication. Analogous to a bending optical fiber [30], it is interesting to explore whether or not the curved graphene waveguide can have application prospects in nano-sized integrated systems and electronic interferometry.

In this article, we investigate the electronic transport properties of curved graphene waveguides by employing Green’s function techniques. Graphene waveguides can be readily prepared by applying an external electric gate along a finite-sized graphene nanoribbon within the graphene flake. We systematically investigate the dependence of the confined waveguide modes on the potential difference \( \Delta V \), the width of waveguide \( W_G \) and the width of the side barrier \( W_B \). It shows that the electronic structures are insensitive to the variation of the width of side barrier \( W_B \). Tunable graphene waveguides can be realized by adjusting the external gate voltage. Through a two-terminal electronic transport calculation, we find that the nearly quantized conductance (ballistic transport) is quite robust against the bending degree of waveguide, in consistence with the band insensitivity to the width of side barrier. In present work, we have observed the signature of valley transport for ultra-thin graphene waveguide with armchair edge. Our findings strongly demonstrate the possibility of designing the graphene-waveguide based low-power nanoelectronics.

### 2. Tight-binding model

In our studies, we consider the armchair graphene nanoribbons, where valleys \( K \) and \( K' \) are mixed and indistinguishable. Figures 1(a) and (b) display respectively the schematic plots of straight and curved graphene waveguides, where the confined potential \( \Delta V \) is applied at the blue colored atomic sites.

![Figure 1](image)

**Figure 1.** Schematic plots of (a) straight and (b) curved waveguides in armchair graphene nanoribbons, being connected with left and right leads extended from the waveguides. Blue atoms label the graphene waveguide. \( W, W_G, W_B \) and \( W_R \) indicate the widths of graphene nanoribbon, left or right terminals, waveguide and side barriers, respectively. \( L \) represents the device length. \( \Delta V \) is the potential difference between waveguide and barriers, and \( V_0 \) is the on-site potential in both side barriers. \( D_c \), the relative shift between left and right terminals, characterizes the degree of bending in curved waveguides.

The \( \pi \)-orbital tight-binding model Hamiltonian of graphene in the presence of gate voltage can be written as:

\[
H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j + \sum_i \tilde{\nu}_i a_i^\dagger a_i, \tag{1}
\]

where \( a_i^\dagger \) and \( a_i \) are the creation and annihilation operators at \( i \)th atomic site, respectively. \( \tilde{\nu}_i \) is the on-site potential energy, which is set to be zero for reference at the side barrier region and \( \Delta V \) in the waveguide region. The nearest-neighbor hopping energy is set to be \( t = 2.78 \) eV. Due to the relatively large width of the system considered, extra Hamiltonian modification for the edge states or other imperfections is not included [32, 33].

### 3. Band structure of graphene waveguide

Band structure can usually provide fundamental information to understand the electronic transport properties. By exactly diagonalizing the tight-binding Hamiltonian of the graphene nanoribbon, the band structure can be obtained. Figure 2(a) displays the band structure of armchair ribbon with a well-known conic-shape subbands encapsulated in the celebrated Dirac conicband of bulk graphene \( E(k_x) = \pm \hbar v_F |k_x| \).

In the standard convention, AGNRs can be defined by N-AGNR where N is the number of dimer lines. Based on crystal structure of graphene, N is related to the width of AGNR, \( W \), via \( W = N \sqrt{a} \), where \( a = 0.142 \) nm is the carbon–carbon bond length. Throughout of this work we employ this relation to establish a connection between different widths and dimer lines which are essential inputs for the numerical code. Here, each supercell includes 818 atoms, corresponding to a width about \( W = 50.4 \) nm. By applying a
gate voltage of $\Delta V = -0.25$ eV at the region of $W_G = 10.1$ nm inside the armchair ribbon, a graphene waveguide is produced and the resulting bands are displayed in figure 2(b). One can observe that the confined modes in blue arise and their mixture with the valence bands result in the asymmetry between the conduction and valence bands in the low-energy region. In below, we show that they are localized inside the graphene waveguide.

Then, we investigate the evolution of confined waveguide modes as a function of the applied gate voltage $\Delta V$. Figure 2(c) displays the first conduction subband variation along with the increase of $\Delta V$. One can find that for a relatively small potential, e.g. $\Delta V = -0.10$ eV, the first conduction subband moves downward; for large potentials exceeding the critical point, e.g. $\Delta V = -0.25$ eV and $-0.35$ eV, the first conduction band becomes overlapped with the valence bands, leading to a band inversion. Figure 2(d) displays the evolution of the first conduction band for different waveguide thicknesses $W_G = 6.1, 10.1, 20.2$ nm and a smooth edge waveguide with full width half maximum (FWHM) being equal to $W_G$, as displayed in upper panels of figures 4(a) and (b). One can find that for narrower waveguide, the band inversion occurs at the position close to the charged neutrality point while for wider waveguide, the band inversion occurs at the energy farther away from the charged neutrality point, therefore giving rise to a wider energy interval for ballistic transport. Figure 2(e) displays the dependence of the first conduction band on the width of the side barrier $W_B$. One can clearly observe that the confined waveguide modes are insensitive to the variation or asymmetry of the width of side barrier $W_B$ (see inset of the panel (e) for magnification of small variation). Therefore, our exploration in figure 2(e) indicates that the confined subbands are insensitive to the ribbon width, beyond the dispersive area with the conduction subbands exhibiting negative slopes. This suggests the possible existence of perfectly conducting (i.e. ballistic transport) energy channels in a graphene waveguide subjected to proper potential wells.

To show how the waveguide modes are distributed in the potential well, in figure 3 we plot the spatial wavefunction distribution across the armchair ribbon at different wavevectors for the four subbands labelled in figure 2(b). For clear comparison, two horizontal white color dashed lines are inserted to identify the boundaries of the quantum well or waveguide. Surprisingly, one can clearly see that most of the confined waveguide modes for wave vectors away from $k_x = 0$ are perfectly confined inside the waveguide; while the remaining parts are not localized inside the waveguide but distributed in the whole range of the ribbon. This is distinct from the topologically protected edge modes that are completely localized at the system boundaries therefore robust against various external disorders.

In a practical device, the potential well across an armchair supercell, a cross-section on transverse direction of figure 1, is usually not a perfect hard-wall profile and often exhibits certain smooth variation between the barrier and the well [15]. Thus, it is essential to characterize conducting energy channels in the presence of edge smoothness. For comparison, two types of potential profiles have been considered: a wider hard-wall waveguide of $W_G = 20.2$ nm and a smooth edge waveguide with full width half maximum (FWHM) being equal to $W_G$, as displayed in upper panels of figures 4(a) and (b). The corresponding band structures are plotted in lower panels of figures 4(c) and (d). Comparison between band structures reveals that waveguide modes do not change substantially when a hard-wall potential profile is replaced by a soft edge potential well. Moreover, we also plot the waveguide modes...
for a supercell system with $W = 80.7 \text{ nm}$ and $W_G = 40.3 \text{ nm}$ in figure 5. Waveguide modes are plotted for two different depths of potential well, namely $\Delta V = -0.25 \text{ eV}$ and $\Delta V = -0.13 \text{ eV}$ in figures 5(a) and (b), respectively. The edge of potential is smooth as plotted in figure 4(b). The waveguide bands are highlighted in blue, and degenerate bands are separated by solid and dashed lines. In the following section, we try to understand the transport properties in a wider graphene nanoribbon by analyzing the conducting bands of a wider armchair supercell. Consequently, we observe that the wider waveguides provide more conducting channels, and the valley degeneracy is still preserved.

4. Electronic transport in curved waveguides

To explore the robustness of the confined waveguide modes against the bending degree of the graphene waveguide, we use a two-terminal mesoscopic setup to study the conductance as a function of the Fermi level $E_F$ for different bending degrees $D_C$. The two terminal conductance $G(E)$ is expressed as

$$G = \frac{2e^2}{h} \text{Tr} [\Gamma L G^* \Gamma R G],$$

where $\Gamma_{L,R}$ are the line-width functions coupling the left and right terminals with the central scattering region [31]. Here, the coefficient ‘2’ represents the spin degree of freedom. The retarded Green function $G^*$ is defined as $G^* = [(E + i\eta) - \mathbf{H} - \Sigma_L - \Sigma_R]^{-1}$ with $G^* = (G^T)^\dagger$. The open boundary condition of the left and right terminals is implemented via $\Gamma_{L,R} = i(\Sigma_{L,R} - \Sigma_{L,R}^*)$, where $\Sigma_{L,R} = (\Sigma_{L,R}^*\Sigma_{L,R})^{1/2}$. Terms $\Sigma_{L,R}$ are respectively self-energies of the semi-infinite left and right terminals [34, 35]. To effectively examine the robustness of the confined waveguide modes of the curved graphene waveguide, one has to ensure that the terminals can better match the central scattering region to avoid the strong back-scattering.

4.1. Tuning external terminals

We first consider both left and right terminals to be exactly extended from the waveguide region to separate the barriers from the terminals physically as displayed in figure 1. The length and width of the graphene ribbon system are respectively set to be $L = 80.7 \text{ nm}$ and $W = 50.4 \text{ nm}$. The waveguide width is chosen to be $W_G = 10.1 \text{ nm}$ and the applied potential is $|\Delta V| = 0.25 \text{ eV}$. There are two reasons for considering the 10.1 nm width waveguide. (a) We are interested in studying the transport on a waveguide with few conducting channels. This might be beneficial in experimental realization since it reduces the scattering among conducting channels and it will enhance the coherent transport. (b) Computational capacity is the other reason. For instance, in our consideration of a 50.4 nm × 80.7 nm central region, a general Green’s function matrix would roughly have $[(50.4/0.5/3\Delta_0) \times (80.7/3\Delta_0)]^2 \approx (409 \times 172)^2$ elements, where $\Delta_0 = 0.142 \text{ nm}$ is the distance between two atoms. This means that it is unrealistic to consider further larger system setups.

In our study, we have done a series of numerical calculation to explore the possibility of realizing quantized conductance, i.e. vanishing backscattering. In figure 6(a), we set the site potentials in the left and right terminals to be identical, i.e. $V_{L/R} = -0.10 \text{ eV}$ or $-0.20 \text{ eV}$. For $V_{L/R} = 0.10 \text{ eV}$, one can find that the first plateau appears around $G = 1(2e^2/h)$, while for $V_{L/R} = 0.20 \text{ eV}$, the first plateau becomes roughly to be $G = 2(2e^2/h)$. However, the presence of same site potential on both left and right terminals always gives rise to an oscillating conductance due to the possible mismatch between the terminals and central scattering region. Surprisingly, we find that if the non-zero site potential is only included in one terminal (e.g. left), plateaus, i.e. $G = 1/3S(2e^2/h)$ arise at different energy intervals (see figure 6(b)). One may ask what would happen to the conductance if $V_L$ and $V_R$ are vanishing? As a sharp comparison, in figure 6(c), we plot the conductance
as a function of Fermi-energy at vanishing site-potentials in both terminals. One can clearly see that the quantized plateaus become oscillating again. This finding emphasizes the importance of the adjustment of site-potentials in both terminals.

4.2. Transport in narrow curved waveguides

Figure 7(a) displays the two-terminal conductance as a function of Fermi level for a curved waveguide with different bending degrees $D_C = 0.0, 10.2, 20.4$ and $30.6$ nm. One can see that for the straight graphene waveguide at $D_C = 0.0$ nm and $E > 0$, the conductance can be approximately quantized to $G = 1, 3, 5(2e^2/h)$. However, for $E < 0$, the conductance becomes oscillating and always be smaller than $G = 1(2e^2/h)$ due to the strong interference between incoming and backscattering modes. It is noteworthy to mention that different site potentials of $V_L = -0.22$ eV and $V_R = 0.00$ eV are applied to the left and right terminals to match the waveguide modes. Here, the odd quantized conductance plateau is determined by the incoming modes from the terminals (see dashed lines in figure 7(c)). When the graphene waveguide gradually becomes smoothly curved (see the lower three panels of figure 7(a)), one may expect backscattering is introduced to break the quantization of conductance. To our surprise, the plateau of $G = 1(2e^2/h)$ is not destroyed even at a higher degree of bending (i.e. $D_C = 30.6$ nm), and it becomes even more flat. This striking transport phenomenon reflects precisely the zero bend resistance, which may be attributed to the immunity of the confined waveguides to the variation of the width of side barriers and can pose immediate implications in graphene-based low-power electronics. The conductance is varying in discrete quanta of $2(2e^2/h)$ in figure 7(a) for second and third plateaus. This indicates the possible valley polarization of conductance due to the imbalanced contribution from different valleys $K$ and $K'$.

In figure 7(b), as an example, we plot the local density of states of the perfectly conducting confined waveguide mode of $G \sim 1 (2e^2/h)$ at fixed $E_F = 0.03$ eV and $D_C = 20.4$ nm. One can see that the confined waveguide mode only propagates locally inside the waveguide. The oscillation peaks on the waveguide are attributed to the traveling wavepackets across the waveguide from the left to right leads. In addition, the number of wavepackets increases at higher Fermi energies, satisfying the plane wave explanation of electron wave function in the transport direction.

Figure 7(c) shows the band matching between the terminals and central scattering region for figure 7(a). As
mentioned, additional site potentials of $-0.22 \text{ eV}$ and $0.00 \text{ eV}$ are respectively added to the terminal’s Hamiltonian to align to similar conduction subbands. For a specific system parameters, careful adjustment of $V_L$ and $V_R$ should be adopted to achieve smooth conductance plateaus, i.e. leads should inject and collect electron effectively. Furthermore, nearly identical conductances at different curvature degrees demonstrate the zero bending resistance of the graphene waveguide as a striking physical property of scattering area. With the increase of $E_F$, the number of bands also increases. The resulting local density of states is no longer perfectly propagating as that in figure 7(b), but accompanying with dispersive distribution over the whole scattering area. However, the restriction of the width of both terminals ensures the full backscattering of the modes spreading in the whole region and only allows the matched propagating modes, giving rise to different ballistic transport plateaus.

We also examined a Gaussian-shape waveguide at a more extended device $L = 131.1 \text{ nm}$ with smooth edges potential well, see figure 8. Relatively similar conductance is achieved. This is in contrary to a recent report claiming an armchair graphene waveguide with smooth edges potential [29]. Thus, we performed the transport study on a straight graphene waveguide [29] utilized a split gate design. The conductances are noticeably smooth at $W_G = 20.2 \text{ nm}$ as compare to $W_G = 10.1 \text{ nm}$. The conductances are not varying in discrete quanta of $2(2/e^2/h)$. Further exploration shows our nanoribbon contacts in figure 9 are semiconductor type nanoribbons while we have used metallic type nanoribbon by far in all of past examples. It is worth mentioning that with ‘$m$’ being an integer number, a nanoribbon with an index number of $3m$ or $3m + 1$ is a semiconductor but $3m + 2$ is a metallic nanoribbon.

It is well known that the current state-of-the-art experiment on graphene waveguide [29] utilized a split gate design. The distance between two top gates was about 121.0 nm and the effective channel width was estimated to be 65.5 nm. Although it is impossible to produce 10.1 nm or 20.2 nm wide lithographic top gates in a realistic device fabrication, one can turn to apply special high-resolution etching techniques [28]. Thus, we performed the transport study on a straight graphene waveguide with $W_G = 40 \text{ nm}$. Results have been plotted in figure 10 and rest of parameters are as follows: $L = 121.0 \text{ nm}$, $W = 100.8 \text{ nm}$, $\Delta V = -0.25 \text{ eV}$, $V_0 = 0.00 \text{ eV}$, $V_L = -0.24 \text{ eV}$ and $V_R = 0.00 \text{ eV}$. Once again, the conductance of the straight and curved waveguides are almost identical. Therefore, the property of zero bending resistivity is independent of the width of graphene waveguide. The conductances are noticeably smooth at $W_G = 20.2 \text{ nm}$ as compared to $W_G = 10.1 \text{ nm}$. The conductances are not varying in discrete quanta of $2(2/e^2/h)$. Further exploration shows our nanoribbon contacts in figure 9 are semiconductor type nanoribbons while we have used metallic type nanoribbon by far in all of past examples. It is worth mentioning that with ‘$m$’ being an integer number, a nanoribbon with an index number of $3m$ or $3m + 1$ is a semiconductor but $3m + 2$ is a metallic nanoribbon.

4.3. Transport in wide waveguides

To highlight the effect of the width of the waveguide, we have considered two example of thicker graphene waveguides, $W_G = 20.2 \text{ nm}$ and $W_G = 40.3 \text{ nm}$. In bandstructure section, we have shown that wider waveguides, with the same amount of potential at the bottom of well, results in more conducting channels with less energy separation. Consequently, It is expecting to have more plateaus with less energy separation. This is confirmed in figure 9 which in there, we have calculated the conductance of medium size graphene waveguide with $W_G = 20.2 \text{ nm}$. Other parameters are as follows: $L = 121.0 \text{ nm}$, $W = 80.7 \text{ nm}$, $\Delta V = -0.25 \text{ eV}$, $V_0 = 0.00 \text{ eV}$, $V_L = -0.24 \text{ eV}$ and $V_R = 0.00 \text{ eV}$. Once
a narrow graphene waveguide. In other word, higher effective mass gives rise to resistivity and leads to a slope between each semi-flat plateaus. Our results agree well with the recent experimental reports [29]. We also observed that decreasing the width of the contacts has a destructive influence on the conductance of a narrow waveguide. When the width of contacts in a waveguide with WG = 10.1 nm is reduced by 25% (about 20 atoms), then the resulting conductance of this waveguide becomes fluctuating, similar to that shown in figure 6(c). As a comparison, in figure 10, we show that a wider waveguide is more immune to the lead-waveguide mismatch.

To better understand the conductance of the wider graphene waveguides, we also plot three other conductances with metallic terminals in figure 11. To make the terminals metallic, we only decrease two atoms in contacts or reduce the index number by one. For example, we choose a straight and a metallic, we only decrease two atoms in contacts or reduce the width of the contacts has a destructive influence on the conductance of a narrow waveguide. When the width of contacts in a waveguide with WG = 10.1 nm is reduced by 25% (about 20 atoms), then the resulting conductance of this waveguide becomes fluctuating, similar to that shown in figure 6(c). As a comparison, in figure 10, we show that a wider waveguide is more immune to the lead-waveguide mismatch.

Figure 10. Conductance of a wider WG = 40.3 nm and straight graphene waveguide with semiconductor type contacts. Rest of device parameters are as follows: L = 120 nm, W = 100.8 nm, ΔV = −0.25 eV, V0 = 0.00 eV, V1 = −0.24 eV and V2 = 0.00 eV. Inset figures show the structure of waveguides. Smoothness is included and color bar shows the on-site potentials.

Figure 11. Conductance of two medium sizes WG = 20.2 nm waveguides and a much thicker WG = 40.3 nm straight graphene waveguide with metallic terminals. For WG = 20.2 nm waveguides we have used the parameters of figure 9 and for single WG = 40.3 nm waveguide we have applied the parameters from figure 10, the case of reduced size. ‘S’ and ‘C’ refer to straight and curved waveguides respectively.

5. Summary

To conclude, we theoretically investigate the electronic transport properties of the confined waveguide modes in curved graphene waveguide. We first systematically study the dependence of the confined waveguide mode on different system geometric parameters and applied gate potentials. We find that the width and symmetry of the side barriers do not affect the bands of the confined waveguide modes, which is a hallmark for the possible ballistic transport in a graphene waveguide with a random but smoothly varying bending. Furthermore, the electronic transport calculation gives direct evidence of nearly quantized conductance in curved graphene waveguide. Such a striking zero bend resistance property makes graphene waveguide an ideal platform to design dissipationless or low-power electronic devices.

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