A gate-induced switch in zigzag graphene nanoribbons and charging effects

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Abstract

Using the non-equilibrium Green’s function formalism, we investigate nonlinear transport and charging effects of gated graphene nanoribbons (GNRs) with an even number of zigzag chains. We find a negative differential resistance (NDR) over a wide range of gate voltages with an on/off ratio $\sim 10^6$ for narrow enough ribbons. This NDR originates from the parity selection rule and also prohibition of transport between discontinuous energy bands. Since the external field is well screened close to the contacts, the NDR is robust against the electrostatic potential. However, for voltages higher than the NDR threshold, due to charge transfer through the edges of the zigzag GNR (ZGNR), screening is reduced such that the external potential can penetrate inside the ribbon giving rise to smaller values of off-current. Furthermore, the on/off ratio of the current depends on the aspect ratio of the length/width and also edge impurity. Moreover, the on/off ratio displays a power law behavior as a function of ribbon length.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Graphene is an intriguing new material, which has been studied extensively since Novoselov et al [1] fabricated it by micromechanical cleavage in 2004. In fact, the flat structure of graphene makes its fabrication more straightforward than carbon nanotubes. Moreover, dreams of carbon nanoelectronics approach reality based on planar graphene structures. This structure overcomes some difficulties of nanoelectronics based on carbon nanotubes, by using lithography, one-dimensional ribbon patterns on graphene sheets [2]. For achieving realistic nanoelectronic applications based on graphene nanoribbons (GNR), the widths of the ribbons have to be narrow enough that a transport gap is opened [3–5]. Sub-10-nm GNR field-effect-transistors with smooth edges have been obtained in [4] and demonstrated to be semiconductors with a band-gap inversely proportional to the width and on/off ratio of the current up to $10^6$ at room temperature.

The origin of the transport gap which is opened in a gate voltage region of suppressed nonlinear conductance is still not well understood [5–7]. Based on the tight-binding approach, GNRees with armchair shaped edges are either metallic or semiconducting [6, 8–10]. Moreover, in this approach, zigzag edge ribbons are metallic regardless of their widths [11]. In contrast, ab initio calculations [6] predict that regardless of the shape of the edges, GNRs are semiconducting. Two factors are responsible for the transport gap: the edge disorder leading to localization [12] and the confinement [8–11]. However, in the nonlinear regime, the transport gap is also opened by transition selection rules which originate from the reflection symmetry [13].

Similar to carbon nanotubes, electronic transition through ZGNRs follows some selection rules. The rotational symmetry of the incoming electron wavefunction with respect to the tube axis is conserved while passing through nanotubes [14]. Correspondingly, the transverse reflection symmetry of the incoming and outgoing wavefunctions results in the parity conservation in ZGNRs with an even number of zigzag chains [13, 15–19]. As a consequence of the even–odd effect, a negative differential resistance (NDR) region appears in the $I–V$ characteristic curve of P–N even ZGNR junctions [19]. A similar NDR behavior has also been reported in P–N nanotube junctions [14]. Historically, NDR was first observed in the degenerated N–P diode junctions [20]. Nowadays, NDR has been reported in many other molecular devices [21, 22].

Motivated by the work done in [4], in this paper, we investigate nonlinear transport through gated even ZGNRs by...
using the non-equilibrium Green’s function (NEGF) approach. The NDR region with an on/off ratio of the current up to $10^6$ appears in the current–voltage characteristic curve. This NDR is induced by transport gaps which are opened by two selection rules governing electron transition through ZGNRs: (i) the parity conservation, and (ii) that allowed transition are between connected bands [15]. Based on band structure analysis, we show that the transport gap opened by the second selection rule is filled for ribbons wider than 10 nm. So, sub-10-nm ribbons with a long enough length provide an experimental manifestation of the NDR phenomenon in the $I–V$ curve of GNRs. On the other hand, the gate voltage regulates the current by shifting the blocked energy regions with respect to the Fermi level. Moreover, the on/off ratio of the current displays a power law behavior as a function of ribbon length as $M^{1.5}$.

Our calculations show that the details of the electrostatic potential profile along the ribbon cannot affect the emergence of NDR. The same conclusion has been reported by [19], but they have not elaborated on the physical reason behind this robustness. By following the self-consistent charge and potential profiles at different voltages, we demonstrate that at low voltages, strong screening of the external potential at contacts results in a flat electrostatic potential along the ribbon. Subsequently, the e–e interaction at a mean field level does not change the magnitude of $I_{on}$. However, for voltages higher than the NDR threshold $V_{on}$, the transfer of charge along the edges leads to a further reduction in $I_{off}$ which improves the switch performance.

This paper is organized as follows: although the formalism has been presented elsewhere [22], for completeness, we briefly introduce the Hamiltonian and NEGF formalism in section 2. In section 3, we discuss the selection rules governing even ZGNRs. The origin of NDR seen in the $I–V$ curve is explained in section 4. We demonstrate in section 5 that the e–e interaction does not have a significant effect on the phenomena of NDR in the $I–V$ curve. Section 6 concludes our results.

2. Hamiltonian and formalism

Figure 1 shows a schematic side view of a graphene nanoribbon. In the presence of a source–drain applied potential, the ribbon is divided into three regions: left, right electrodes and also a central interacting region. The gate voltage is applied by means of the substrate on the graphene plate. The interacting Hamiltonian governing the electron dynamics is written in the tight-binding approximation. This Hamiltonian is a functional of charge density:

$$H [n] = \sum_i \left( \varepsilon_i + \frac{(x_i-x_0)/L - 0.5 |V_{sd}|}{|V_{sd}|} \right) c_i^\dagger c_i + \sum_{ij} t (c_i^\dagger c_j + c_j^\dagger c_i),$$

(1)

$\varepsilon_i$ shows the on-site energy of the $i$th carbon atom and $t$ represents the hopping integral between nearest neighbor atoms. One $\pi$ orbital is considered for each site for the graphene system. Without losing any generality, we set the on-site energies ($\varepsilon_i$) of all sites equal to zero. All energies are in units of $t_{C-C} = 2.5$ eV. The application of a gate voltage is achieved by shifting the atomic on-site energies in all three regions. The applied source–drain potential, $V_{sd}$, and the gate voltage, $V_g$, preserve the transverse symmetry with respect to the ribbon axis ($X$ direction in figure 1). Linear variation of the source–drain voltage along the ribbon is the solution of the Laplace equation with the Dirichlet boundary condition on the contacts. $U_{ij}$ is the electrostatic Green’s function and $\delta n_i = n_i - n_0$ is the change in the self-consistent charge $n_i$ from its initial equilibrium zero-bias value. This third term is the direct Coulomb interaction created by the bias-induced charges at a mean field level which is the solution of the Poisson equation. The electrostatic Green’s function for a distribution of charges between two parallel conducting planes located at $x = 0, L$. 

![Figure 1. Gated zigzag graphene nanoribbon which is divided into three regions: left, right and central region. The dotted rectangular region is the unit cell which is used for finding the band structure of graphene ribbons. The lower panel shows a field-effect transistor structure based on graphene ribbons where the gate voltage is applied on the whole system.](image-url)
which are held at zero potential [24], has the following form:

\[ U(\vec{r}, \vec{r}') = 2 \int_0^\infty dk J_0(ak) \frac{\sinh(k(z_2 - z_1))}{\sinh(kL)} \frac{\sinh(k(L - z_1))}{\sinh(kL)} \]

\[ \alpha = \sqrt{(x-x')^2 + (y-y')^2 + U_H^2}, \]

where \( U_H \) is the Hubbard parameter whose semi-empirical value for carbon [25] is about \( 4t_{C-C} \). This parameter determines the strength of the electron–electron interaction. This electrostatic Green’s function is appropriate for the kernel of the Ohno–Klopman model [26].

First of all, we must find the self-consistent charge and electrostatic potential by using the NEGF formalism. The retarded and advanced Green’s function matrix subjected to the central portion of the ribbon is as follows:

\[ G^{\pm\pm}(E, n) = [(E \pm \eta)I - H[n] - \Sigma_L^{\pm} - \Sigma_R^{\pm} + \Gamma_1^{\pm\pm} - \Gamma_1^{\pm\pm}], \]

where \( \eta \to 0^+ \). ‘I’ is the unit matrix. \( \Sigma_L^{\pm}, \Sigma_R^{\pm} \) are the retarded self-energies due to scattering by the left/right electrodes. These self-energies are independent of the charge density. To determine the self-energy, one needs to calculate the surface Green’s function of semi-infinite electrodes \( g_p(E) \) by using the Lopez–Sancho’s method [27]. Having Green’s function, one can find the total charge \( n = n^{\text{eq}} + n^{\text{non-eq}} \) by separate calculations of the equilibrium and non-equilibrium charges by using the retarded and lesser Green’s functions, respectively. It is simply demonstrated that in the coherent regime, the lesser Green’s function can be represented by the retarded and advanced Green’s functions which are determined in equation (3).

\[ n_i^{\text{eq}} = -\frac{1}{\pi} \int_{\mu_v - V_{sd}/2}^{\mu_v + V_{sd}/2} \text{Im}[G_{ii}^{\prime}(E)] dE, \]

\[ n_i^{\text{non-eq}} = \frac{1}{2\pi} \int_{\mu_v - V_{sd}/2}^{\mu_v + V_{sd}/2} [G^{\pm\pm}(\Gamma_1 L, \Gamma_1 R) G^{\text{eq}}]_{ii} dE, \]

where \( f_p = 1/[1 + \exp(E/E_{Fp})] \) shows the Fermi function of the electrodes, and \( \mu_0 = \mu_R = \mu_L \) show electrochemical potentials of the left and right electrodes. The initial charge \( n_i^{\text{eq}} \) is calculated by the equilibrium integration in zero bias. To obtain the charge, coupled equations of (1) and (3) are self-consistently solved by using Broyden’s method [28]. The transmission coefficient \( T(E, V) \) is defined in terms of self-consistent Green’s functions as:

\[ T = \text{Tr}[G^\dagger \Gamma_R G^2 \Gamma_L]. \]

The current passing through the nanoribbon is calculated by the Landauer formula at zero temperature [29]:

\[ I(V) = \frac{2e}{h} \int_{\mu_v - V_{sd}/2}^{\mu_v + V_{sd}/2} dE T(E, V). \]
variations. The electronic transition between an eigenstate

$$k_x$$

width of the central bands at

$$S$$

ZGNRs and the parity of band

$$m$$

(upper/lower group of bands from the central bands at the Dirac point

$$q$$

g = ± 0 V

$$V$$

2

= ± 13

$$γ$$

$$k$$

is so large that one can assume

$$V_{sd}(k − q) → δ(k − q).$$

Therefore, a smooth potential in the longitudinal direction can just scatter the electron among the class of states belonging to the same group of connected energy bands.

Now let us focus on the two transport gap regions: AB and CD in figure 2(b). The AB gap is a consequence of parity selection rules, while the CD gap is due to blockage of the transition between disconnected groups. As can be seen in figure 2(b), the AB gap is proportional to the source–drain voltage, $V_{sd}$. Moreover, this gap is independent of the ribbon width. Of course, in wide ribbons, upper and lower band groups approach the central group, especially at point $k_z = 0$, where $γ$ in figure 2(a) tends to zero as log-normal.

When the ribbon width is increased, the separation $γ$ between the upper/lower and central groups of bands is reduced, which tends to loosen the second selection rule based on band groups; hence filling in the gaps. However, when we increase the ribbon length, our classification of bands into connected groups is recovered. Therefore, the AB gap is essentially governed by the aspect ratio of the ZGNR.

The CD gap is equal to $Δ − δ + V_{sd}$, where $Δ$ and $δ$ are the energy separation of the upper/lower group from the central bands at the Dirac point ($k_z = ±2π/3a$) and $k_z = 0$, respectively. Moreover, $δ$ is the half width of the central bands at $k_z = 0$.

Figure 2. Transmission (right panel) and band structure of the right (center panel) and left (left panel) electrodes for a ZGNR with six unit cells in length and four zigzag chains. The applied bias is considered to be (a) $V_{sd} = 0$ and (b) $V_{sd} = 1.0$. The gate voltage is $V_g = 0.5$ V. Here, $Δ$ and $γ$ are the energy separation of the upper/lower group of bands from the central bands at the Dirac point ($k_z = ±2π/3a$) and $k_z = 0$, respectively. Moreover, $δ$ is the half width of the central bands at $k_z = 0$.

boundary, while distinct groups are disconnected. When one considers the electron transport, the longitudinal momentum $k_z$ of electrons changes as a result of applied $V_{sd}$. The precise form of this variation in $k_z$ crucially depends on the profile of the superimposed longitudinal potential. These groups are disconnected from each other from the point of longitudinal momentum. The transport properties for smoothly varying $V_{sd}$ are significantly different from $V_{sd}$ profiles with sharp spatial variations. The electronic transition between an eigenstate $(m_1, k)$ in the right electrode and an eigenstate $(m_2, q)$ in the left electrode is proportional to Fourier transformation of the longitudinal voltage and structure factor [15].

$$\langle ψ_{m1}(k) | V_{sd}(x) | ψ_{m2}(q) \rangle = S V_{sd}(k − q) \delta,$$ (7)

where structure factor $δ$ is equal to $[1 + (−1)^{P_{m1} + P_{m2}}]$ for even ZGNRs and the parity of band $m$ is equal to $P_m = (−1)^{m+1}$. The parity selection rule in even ZGNRs originates from this structure factor. This parity selection rule is a mesoscopic analog of the chirality factors governing the transport of Dirac electrons in planar graphene [23].

In our calculations, we apply a constant gate voltage to the whole system without any longitudinal variation. As a result, the gate voltage does not change the momentum of the electron. However, linear variation of the applied source–drain bias (with the slope $V_{sd}/L$) changes the electron momentum. Therefore, smooth variation of the potential in longer ribbons results in a small momentum variation of the electron. Consequently, transition of the electron between disconnected bands is forbidden when the length of the ribbon is so large that one can assume $V_{sd}(k − q) → δ(k − q)$. Therefore, a smooth potential in the longitudinal direction can just scatter the electron among the class of states belonging to the same group of connected energy bands.

NDR threshold voltage on the gate voltage can also be seen in figure 2(b), the AB gap is a consequence of parity selection rules, while the CD gap is due to blockage of the transition between disconnected groups. As can be seen in figure 2(b), the AB gap is proportional to the source–drain voltage, $V_{sd}$. Moreover, this gap is independent of the ribbon width. Of course, in wide ribbons, upper and lower band groups approach the central group, especially at point $k_z = 0$, where $γ$ in figure 2(a) tends to zero as log-normal.

When the ribbon width is increased, the separation $γ$ between the upper/lower and central groups of bands is reduced, which tends to loosen the second selection rule based on band groups; hence filling in the gaps. However, when we increase the ribbon length, our classification of bands into connected groups is recovered. Therefore, the AB gap is essentially governed by the aspect ratio of the ZGNR.

The CD gap is equal to $Δ − δ + V_{sd}$, where $Δ$ and $δ$ are the energy separation of the upper/lower group from the central bands at the Dirac point, and the half width of the central bands at $k_z = 0$, respectively. The dependence of $Δ$ on width $N$ is: $Δ ∝ (2.13 ± 0.02)N^{−(0.864±0.003)}$, while $δ$ has a log-normal behavior which asymptotically approaches the constant value of 0.9738 ± 0.0002 as $N$ goes up to 10. The conducting region BC in figure 2(b) can exist only when $Δ − δ < V_{sd} < δ$. From the dependence of $Δ$ and $δ$ on $N$, the CD gap exists if $N$ is less than 30. Hence, NDR is estimated to be observable for a ribbon width ≤ 7 nm. The lowest achieved ribbon width is sub-10-nm wide (~2 ± 0.5 nm) [4] with the length ~236 nm. Such long ribbons with small widths provide a fascinating experimental manifestation of the selection rules in transport properties.

4. Negative differential resistance

Figure 3 shows the current–voltage characteristic curve of a ZGNR with four zigzag chains and six unit cells in length. In the case of zero gate voltage, the flow of current is blocked due to the parity selection rule, while at a given $V_{sd}$, gate bias turns the current on. After a range of $V_{sd}$ in which the current remains unchanged, the current begins to reduce with increasing $V_{sd}$. The NDR threshold voltage $V_{sd}$ decreases with gate voltage for $V_g < 0.6$ V. The dependence of the NDR threshold voltage on the gate voltage can also be seen in...
nonzero range of transmission remains unchanged along with the current integration window of equation (6). However, the AB, originating from the parity selection rule, contributes to the AB and CD gaps in voltages $V_{\text{bc}}$ in transport is accompanied by the blockage arising from voltages $V_{\text{sd}}$ resulting in the fixed current in the voltage range $[V_{\text{g}}, V_{\beta}]$. Therefore, the current remains unchanged in this range. For voltages $V \geq V_{\beta}$, the CD gap contributes in the current integration window, and consequently the NDR phenomenon emerges.

Regarding the importance of gate voltage in the current flow, let us investigate the effect of the gate voltage on the $I-V_{\text{sd}}$ curve by contour plotting of the current with respect to $V_{\text{sd}}$ and $V_{g}$ in figure 4. For gate voltages $|V_{g}| < 0.1 \text{ V}$, the shift in transmission is not remarkable enough to contribute to conducting channels in the current integration. Therefore, the current is blocked by the parity selection rule. In the range $0.1 \text{ V} < |V_{g}| < 0.6 \text{ V}$, the contribution of conducting region BC in transport is accompanied by the blockage arising from the AB and CD gaps in voltages $V > V_{\text{on}}$. As a consequence, the current reduces after a threshold voltage. In this range, the on/off ratio of the current increases and $V_{\text{on}}$ reduces with increasing gate voltage.

As can be seen in the $I-V$ curves of figure 3, the off-current reduces for longer ribbons which enables us to achieve high performance switches by increasing the aspect ratio of the ribbon length/width. The reason for this is connected to the smooth variation of the applied potential along the ribbon such that during transport, electrons are scattered among those states which belong to continuous bands. As a consequence, blockage originating from electronic transition between disconnected bands is intensified by increasing the ribbon length. In fact, when the length of the ribbon increases, transmission in the AB and CD gaps decreases exponentially.

Since the off-current is induced by the contribution of the gaps in the current integration, $I_{\text{off}}$ efficiently decreases with increasing ribbon length ($M$). Figure 6(a) shows that $I_{\text{on}}/I_{\text{off}}$ displays a power law behavior as a function of the ribbon length for large $M$: $I_{\text{on}}/I_{\text{off}} \propto M^{\eta}$ where $\eta = 7.5061 \pm 0.03505$. As an example, for $M = 50$, the on/off ratio goes up to $10^{6}$.

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**Figure 3.** Current–voltage characteristic curve for different gate voltages when the ribbon size is $(N, M) = (4, 6)$. The effect of different parameters such as the size effect, electrostatic potential and also gate voltage is investigated on the $I-V$ curve. The Hubbard parameter ($U_{\text{H}}$) is on-site Coulomb repulsive.

**Figure 4.** Contour plot of transmission with respect to the energy and $V_{\text{sd}}$ for system size $(N, M) = (4, 6)$ and applied gate voltage $V_{g} = 0.5 \text{ V}$. The dark oblique line shows the current integration window. The points marked by A, B, C, D correspond to the horizontal lines with the same name in figure 2. The lines of $\alpha, \beta$ are the trace of points with similar names in figure 3. The Fermi energy was fixed at zero $E_{F} = 0$.

**Figure 5.** Contour plot of the current in terms of $V_{\text{sd}}$ and $V_{g}$ for a zigzag graphene nanoribbon with $(N, M) = (4, 6)$. The vertical dotted line corresponds to $V_{g} = 0.5 \text{ V}$. $\alpha$ and $\beta$ are those points which were shown in figures 3 and 4.
which suggests experimental fabrication of high performance switches based on the GNR nanoelectronics.

Experimentally, it was observed in [4] that the room temperature on/off ratio induced by the gate voltage increases exponentially as the GNR width decreases. They observed that $I_{on}/I_{off}$ is equal to 1.5, 100, and $>10^2$ for $W = 50$ nm, 20 nm, 10 nm and sub-10-nm, respectively. Similarly, as shown in figure 6(b), the on/off ratio calculated for the set up considered in this paper, also decreases with the ribbon width, while reduction of the on/off ratio can be compensated by considering longer ribbons. However, the NDR phenomenon disappears for ribbons wider than 7 nm.

In ab initio calculations [6], by using hydrogen termination of zigzag edges, the mirror symmetry of ZGNRs and consequently the parity conservation could be retained. Correspondingly, by several repetitions of the heat treatments and hydrogenation, it is also possible to create well-ordered H-terminated edges in experiment [32]. However, edge states with energies about $-0.1$ to $0.2$ eV have been experimentally observed [32] that emerge at hydrogen-terminated zigzag edges. To simulate the edge states and the effect of symmetry breaking on NDR phenomenon, it is assumed to dope one of the ZGNR edges by a slight impurity. Edge impurity is considered to apply as a change in the on-site energy of the edge atoms ($\varepsilon_\alpha$) with respect to the on-site energy of the other atoms. In the case of edge disorder, $\varepsilon_\alpha$ plays the role of the averaged on-site energy of the edge atoms. The inset in figure 6(b) shows that on/off switching reduces with edge impurity strength; however, NDR still emerges for $\varepsilon_\alpha < 0.3\varepsilon_{C-C}$.

5. Electrostatic potential and charging effect on NDR

The emerging phenomenon of negative differential resistance in the $I-V$ curve is not destroyed by the e–e interaction and is independent of the details of the electrostatic potential profile. However, the interaction reduces the off-current as shown in the $I-V$ curves of figure 3. To substantiate the above claim, comparison of transmission curves in the presence and absence of the e–e interaction is useful. It is apparent from figure 7(a) that for voltages less than $V_{on}$, transmission in conducting channels is robust against the e–e interaction while transmission increases in the gaps with respect to the non-interacting case. However, this enhancement is slight enough that it cannot affect the emergence of NDR. However, for voltages $V > V_{on}$, the interaction lowers the transmission coefficient in the conducting channels (such as the BC region) in which higher subbands participate in transport. Such behavior is corroborated in figure 7(b), which indicates transmission at that voltage corresponding to the off-current, $V_{off}$. Reduction in the transmission coefficient of the conducting channels results in a further reduction of the off-current. To explain the reason for such a phenomenon, it is necessary to study the potential and charge profiles. The electrostatic potential averaged on each unit cell is represented in figure 8(a) in terms of the ribbon length. For voltages less than $V_{on}$, the potential sharply drops only at the contact region which connects the system to the electrodes. In such a case, the external potential is strongly screened by redistributed electrons and, the electrostatic potential of the central atoms remains close to zero. Screening is performed by discharging of electrons from the area connected to the source and their accumulation around the drain electrode. These facts are obvious from the transferred charge and electrostatic potential profiles represented in figure 9. Since $U(n-n_0)$ determines the electrostatic behavior of the potential, discharging of electrons weakens the external potential penetrated from the source electrode. Moreover, charge accumulation around the drain electrode prevents potential drop in the central part of the system. Therefore, in the case of strong screening, the potential drops only at the contacts. However, when the applied bias goes beyond 1 V, screening is being weakened and the external potential can penetrate inside the central region. The reason why screening is weak can be sought in charge distribution.
Figure 8. (a) Electrostatic potential per unit cell in terms of unit cell position for source–drain voltages 0.5, 0.75, 1.25 V. (b) Edge, middle and total transferred charge in terms of source–drain applied bias. The gate voltage is for all curves equal to \( V_g = 0.5 \) V.

Figure 9. Transferred charge and electrostatic potential profiles for \( V_{sd} = 1.25 \) V and \( V_g = 0.5 \) V in the weak screening case. Due to charge transfer through the ribbon edges, screening is so weak that the external potential can penetrate inside the central portion.

In summary, at voltages less than \( V_{on} \), the electrostatic potential is only dropped at the contacts and therefore the momentum of the electrons only varies in the area where the potential drops, while the longitudinal momentum of the electrons remains unchanged across the central portion. In other words, the potential steeply drops in the low-area district around the contacts, which results in violation of the blockage rule which governs the transition between disconnected energy bands. Subsequently, the transmission coefficient slightly increases in the blocked energy ranges. In other words, in this case, an increase in the gradient of the potential facilitates electronic transport in the blocked energies. Note that the interaction preserves transverse symmetry, so the parity selection rule still governs electronic transport. Therefore, the AB gap induced by the parity conservation still survives for voltages larger than \( V_{on} \). For voltages \( V > V_{on} \), the electrostatic potential gradually penetrates into the whole system so that the potential of the central region is not flat. In addition, because the edge transport of electrons dominates, the transverse potential is deeper in the middle of the ZGNR than its edges. Therefore, the band structure of the interacting central region differs from the band structure of electrodes. As a consequence, for voltages \( V > V_{on} \), the transmission of conducting channels and also the off-current reduces.

6. Conclusion

In this paper, using the non-equilibrium Green’s function approach, we investigated nonlinear transport and charging effects of graphene nanoribbons with even zigzag chains. The current flow is controlled by the gate voltage applied on the whole of the sub-10-nm ribbons. In this range of widths, two selection rules govern the electronic transition: (i) the parity conservation, and (ii) allowed transition between connected bands. As a result, a negative differential resistance (NDR) in the \( I-V \) curve appears in the presence of the gate voltage. Furthermore, the on/off ratio of the current increases with the ribbon length as a power law behavior up to \( 10^6 \), while ribbon width and edge impurity reduce the on/off ratio. The emergence of the NDR phenomenon is not sensitive to details of the electrostatic potential profile. As a result of strong screening in low voltages, the major potential drop takes place at the contacts. However, for voltages larger than the NDR threshold, due to charge transfer through the ribbon edges, screening is so weak that the external potential can penetrate inside the central portion. As a consequence, the off-current reduces in comparison to non-interacting ribbons.

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