Negative differential resistances with back gate-controlled lowest operation windows in graphene double barrier resonant tunneling diodes

Yu Song,1,∗ Han-Chun Wu,2 and Yong Guo1

1Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, People’s Republic of China
2School of Physics and CRANN, Trinity College Dublin, Dublin 2, Ireland
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We theoretically investigate negative differential resistance (NDR) of massless and massive Dirac Fermions in double barrier resonant tunneling diodes based on sufficiently short and wide graphene strips. The current-voltage characteristics calculated in a rotated pseudospin space show that, the NDR feature only presents with appropriate structural parameters for the massless case and the peak-to-valley current ratio can be enhanced exponentially by a tunable band gap. Remarkably, the lowest NDR operation window is nearly structure-free and can be almost solely controlled by a back gate, which may have potential applications in NDR devices with the operation window as a crucial parameter.

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Electronic address: kwungyusung@gmail.com

Negative differential resistance (NDR) is a fundamental physical phenomenon which has been observed in various systems, including gaseous media, chalcogenide glasses, organic semiconductors, conductive polymers, etc. In electronics, NDR is widely used in high-speed applications including high-frequency signal generation and high-speed switching, and functional applications such as one-transistor static memories and multi-valued memory circuits. Recently, extensive efforts have been devoted to the study of NDR in graphene, a monolayer of $sp^2$ bonded carbon atoms that has attracted much attentions since its discovery. NDR features in graphene single barrier diodes, zigzag nanoribbons, armchair nanoribbons, numerus nanoribbon junctions, armchair superlattices, and three terminal field-effect transistors have been theoretically or experimentally reported.

It is well-known that resonant tunneling (or equivalently Fabry-Pérot-type interference) is a fundamental mechanism for NDR; it plays a dominant role in the NDR feature in common semiconductor based resonant tunneling diodes (RTDs). Surprisingly, so far this basic mechanism has not been explored in graphene except the armchair superlattices work. However, in this structure, other mechanisms (band gaps, miniband conductance, and Wannier-Stark ladder) also contribute to the NDR feature and thus significantly obscure the resonant tunneling mechanism.

In this letter, we theoretically investigate the NDR feature of massless and massive Dirac Fermions in double barrier (DB) RTDs based on sufficiently short and wide graphene strips (see, Fig. 1(a)). We consider a realistic linear voltage drop along the source and drain electrodes (see, Fig. 1(b)) and calculate the current-voltage characteristics in a rotated pseudospin space (see, Fig. 1(a)) within the Landauer-Büttiker formalism. We find that the NDR only appears with appropriate structural parameters for the massless case and the peak-to-valley current ratio can be enhanced nearly exponentially by a tunable band gap. Remarkably, we also find that the lowest NDR operation window (the bias range between the current peak and valley) is nearly free to the structural parameters and is always locked around the Fermi energy hence can be almost solely controlled by a back gate. This phenomenon could be of benefit to NDR devices in which the operation window plays a dominant role.

The structure of the graphene DB RTDs is shown in Fig. 1(a). A graphene strip with a dimension of $L_1 \times W$ is placed on a substrate in the $x$-$y$ plane. Here $W$ is several times of $L_1$ to ensure that the edge effect is negligible. The graphene strip is further contacted by a source and drain electrode along the $y$-direction and isolated by an insulator layer on top of it. When made of high-$\kappa$ (dielectric constant) material, the contact can be regarded as ideal, i.e., the contact-induced energy broadening and a finite contact resistance can be ignored. The DB RTD can be fabricated by patterning two top gates ($V_{t1}$ and $V_{t2}$) on top of the insulator layer along the $y$-direction, and contacting a back gate ($V_{BG}$) to the substrate. The realistic barriers formed by the top gates are smooth due to the interface electric field. However, they can be regarded as rectangular ones with the same lengths but effective heights determined by the smoothness of the realistic barriers. The carrier concentration in the graphene strip is linearly tuned by the back gate. Accordingly the Fermi energy (respective to the graphene charge neutrality point, i.e., the Dirac point $E_D \equiv 0$) is also tuned by the back gate since $E_F \propto \text{sign}(n) \sqrt{|n|}$, when a bias voltage is applied between the source and drain, a linear voltage drop along the $x$-direction will be formed due to a uniform in-plane electric field (see, Fig. 1(b)). Meanwhile, a net current will be produced by the electrons or...
dependent electrostatic potential, and $I_p$ are Pauli’s matrices, operator, $\Delta$ is a tunable band gap (i.e., the mass of the (see, Fig. 1(a)). The Hamiltonian becomes\[23\]
equation. Here we perform a rotation of the Dirac equation. Fortunately results in an unsolvable two-order differential equation. To calculate the I-V characteristics in the Landauer-Büttiker formalism,\[24\] one need to first solve envelope function $\Psi(x,y) = (\psi^+,\psi^-)^T$ where $\uparrow / \downarrow$ corresponds to the A/B sublattice in each uniform region. Straightforward decouple of the original Dirac equation containing the electric field along the $x$-direction, however, unfortunately results in an unsolvable two-order differential equation. Here we perform a rotation of the Dirac equation by $\pi/2$ around the $y$-axis in the pseudospin space (see, Fig. 1(a)). The Hamiltonian becomes\[23\]

$$H = v_F(\sigma_z p_x + \sigma_y p_y - \sigma_z \Delta) + eV(x)I.$$ (1)

Here $v_F \approx 10^6 m/s$ is the Fermi velocity, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli’s matrices, $p = (hk_x, hk_y)^T$ is the momentum operator, $\Delta$ is a tunable band gap (i.e., the mass of the Dirac Fermions) up to several hundred of meV achieved through a controllable doping.\[24\] $V(x)$ is the position dependent electrostatic potential, and $I$ is the 2×2 identity matrix. For convenience we express all the parameters in their dimensionless form: $x = x/l_0$, $k = k_{0}$, $\epsilon = E/E_0$, $\delta = \Delta/E_0$, and $v(x) = eV(x)/E_0$ in terms of a characteristic length $l_0$ and corresponding energy unit $E_0 \equiv h\nu_F/l_0$. $l_0$ is adopted as 40 nm ($E_0 \approx 16.44$ meV) to ensure the electron density of states coinciding with a true system and a coherent transport regime even at room temperature.

The envelope functions in the buffer and well (barrier) regions can be exactly solved from the decoupled two-order differential equation

$$\Psi = p \left( \begin{array}{c} F \\ G \end{array} \right) e^{ik_y y} + q \left( \begin{array}{c} G^* \\ F^* \end{array} \right) e^{ik_y y},$$ (2)

where $F = D[-1 + iq^2/2a_i, (1 + i)(\epsilon + az(-v_i))/\sqrt{a}]$ and $G = (1 + i)\sqrt{a}q^{-1}D[iq^2/2a_i, (1 + i)(\epsilon + az(-v_i))/\sqrt{a}]$ with $D$ being the Weber parabolic cylinder function, $q^2 = k_y^2 + \delta^2$, and $a = eV_b/L$ ($L = 2l_0 + l_1 + d + l_2 < L_t$ is the total length between the source and drain). Note, $F$ and $G$ ($F^*$ and $G^*$) have properties of a right (left-going) wave function.\[23\] The decoupled two-order differential equation in the electrode regions recovers the one before performing rotation. A proper envelope function should be adopted as $\tilde{\Psi}(x,y) = (\psi^+,\psi^-)^T$ with the spinor components relating with the original ones by $\psi^\pm = (\pm \psi^+, \psi^-)/\sqrt{2}$.

The transmission coefficient ($t$) can be obtained by matching the spinor envelope functions at the potential boundaries with the standard transfer-matrix method.\[23\] The transmission probability reads $T = k_{Dx}(\epsilon + \delta)k_{Sx}^{-1}(\epsilon + \delta + v_b)^{-1}|t|^2$ for $k_{Sx}^2 > 0$ and $k_{Dx}^2 > 0$, and $T = 0$ otherwise, where $k_{S(D)x}$ is the value of $k_x$ at the source (drain) electrode. Then the net current at zero temperature can be calculated by the Landauer-Büttiker

\[\text{FIG. 1: (color online) Model construction for I-V characteristics of graphene DB RTDs. (a) The diode contains two barriers (with lengths $l_{1(2)}$ and height $V_{1(2)}$) separated by a well (with length $d$), and two buffer regions (with length $l_b$) separating the barriers and the electrodes. The two rectangular angles show the rotation we make in the pseudospin space. (b) The biased transport can be divided into three regimes defined by the Fermi energy $E_F$, and the finite bias $V_b$. In these regimes, electron-to-electron (I), hole-to-electron (II), and restricted hole-to-electron transport (III) respectively contributes to the DC. In regime I (II) the bias induced DC is approximately proportional to $eV_b (eV_b - E)$ (see, Ref. 13), while in regime III only holes within critical incident angles $\pm \sin^{-1}(1 + eV_b/E)$ contribute to the transport (that’s why we call it restricted).\]
Interestingly, in graphene these suppression regions in Fig. 3(b)) enter the integration window of the ripples with a possible NDR feature around gate. One can see that, the I-V curves display obvious DB RTD at various Fermi energies controlled by the back formalism\[22\]

\[ I(V_b) = I_0 \int_{\epsilon_F-v_b}^{\epsilon_F} \int_{-\pi/2}^{\pi/2} T(\epsilon, \theta, v_b) |e| \cos \theta \, d\theta \, d\epsilon, \]

(3)

where \( I_0 = 4e\nu_F W/(2\pi l_0)^2 \) is a current unit with the factor 4 coming from the spin and valley degeneracies. Calculated current based on Eq. (2) avoids possible nonphysical current induced by a steplike approximation of the voltage drop.\[6, 10\]

\[ \Delta I(\epsilon, \theta, v_b) = \frac{\pi l_0}{2e} \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]

where \( \Delta I \) is a current unit with the factor \( \pi l_0/2e \). For both the graphene and 2DEG cases the differences are the same for (a) gapless graphene and (b) 2DEG. For both the graphene and 2DEG cases the differences are the same for \( \pm \alpha \).

Fig. 2(a) shows the I-V characteristics of a graphene DB RTD at various Fermi energies controlled by the back gate. One can see that, the I-V curves display obvious ripples with a possible NDR feature around \( eV_b = E_0 \). To analyze whether there is a NDR or not, we further plot the differential conductance (DC) in Fig. 2(b). As is seen, when the bias sweeps from zero, the DC first decreases and then increases successively with a relatively big and small gradient. This can be understood by the three transport regimes marked and described in Fig. 1(b). Moreover, one can see clearly the oscillation behavior in DC, which is a result of the alternate enhancement and suppression of \( T \) respectively at and between resonant tunneling peaks (see, Fig. 3(a)). Note, for a given \( E_F \) the DC achieves the minimum (\( G_m \)) at some bias. We summary \( G_m \) as a function of the Fermi energy in the inset of Fig. 2(b). One can see that it first decreases and then increases with increasing \( E_F \). The global minimum DC for the considered structure appears at \( \epsilon_F = 0.9 \) with a value of about 0.013, which confirms that there is no NDR in such a graphene DB RTD.

This is an interesting result comparing with the rather obvious NDR in two-dimensional electron gas (2DEG) based DB RTD with the same structural parameters (see inset in Fig. 2(a)). In this type of RTD’s, NDR occurs when the suppression regions of \( T \) (i.e., blue regions in Fig. 3(b)) enter the integration window of the current.\[14\] Interestingly, in graphene these suppression regions are significantly reduced (see, Fig. 3(a)), especially for relatively small incident angles which unfortunately make the main contribution to the NDR (see the factor \( \cos \theta \) in Eq. (3)). This is because the quasi-bound states (equivalently, resonant tunneling peaks) are hard to form due to the Klein tunneling\[26\] in these regions. Moreover, the integration window in graphene is \([E_F - eV_b, E_F]\) rather than \([\text{Max}(0, E_F - eV_b), E_F]\) in 2DEG or common semiconductors. Here, \( \text{Max}(u, v) \) stands for the bigger one of \( u \) and \( v \). Then when \( eV_b \) exceeds \( E_F \), the hole-to-electron transport in transport regimes II and III (which is absent in the semiconductors case) also contributes a positive DC in the I-V curves of graphene. This DC increases with increasing bias hence further suppresses the NDR feature in graphene. Therefore, the I-V characteristics and NDR features in graphene DB RTDs are a competition of hole-to-electron transport and Klein tunneling with the resonant tunnelings.

The absence of NDR can be overcome by enhancing the resonant tunneling in DB RTDs with more appropriate structural parameters. We find that the less the quasi-bound states (which approximately equals to the value of \( v_t d \)), the stronger the contribution of the resonant tunneling. Fig. 4 shows the I-V characteristics and DC’s for a DB RTD with \( b = 1/2, \) \( l_{1(2)} = 1/2, \) \( d = 1/2, \) and \( v_{1(2)} = 2 \). Along the arrow, \( \epsilon_F = 2.4, 2.6, 2.8, 3.0, \) and 3.2. Insert in (b): the bias positions for the current peak (curve with ▲), valley (▼), and minimum DC (●) as a function of the Fermi energy.

\[ G_m = \frac{\pi l_0}{2e} \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]

\[ \int_{-\pi/2}^{\pi/2} |e| \cos \theta \, d\theta \, d\epsilon, \]

\[ \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]

\[ \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]

\[ \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]

\[ \int_{\epsilon_F-v_b}^{\epsilon_F} |e| \cos \theta \, d\theta \, d\epsilon, \]
els of the quantum well. Then the operation windows (OWs) are almost Fermi energy-free and synthetically controlled by the structural parameters (i.e., $l_{1,2}$, $v_{1,2}$, and $d$). In contrast, for graphene DB RTDs, the central position for the lowest OW is almost structure-free and depends only on the Fermi energy. Then by solely tuning the back gate voltage the Fermi energy and hence the lowest OW can be exactly controlled or chosen as long as the NDR is present.

It is found in Fig. 2(b) that, the biases for local minimum DC's generally decrease with increasing Fermi energy (the one around $v_b = 1.2$ for $eF = 0.7$ is an exception). Note, for $G_{in}$ the bias increases almost linearly as a function of $E_F$. On the other hand, for $eV_b < E_F$ it is purely electron-to-electron transport, while for $eV_b > E_F$ both electron-to-electron and hole-to-electron transports make contribution. So, the ambipolar transport is at the heart of the physics for the remarkable back gate-controlled lowest OW. Note the lower output voltage in high-speed switching circuits and the two stored states in static memory elements are determined exactly by the OW (see Ref. 5 and relevant references therein). Such back gate-controlled OW would have potential applications in these NDR based devices.

The PVR is still rather small (about 1.02 for the strongest case $eF = 2.8$) for these gapless graphene based DB RTDs. In Fig. 5(a) we show the I-V characteristics for graphene DB RTDs with different band gaps. Along the arrow, $\delta = 0$, 0.5, 1.0, 1.5, 2.0, and 2.5 (enlarged by 5 times for clearness). (b) The peak-to-valley current ratio and (c) the biases for the current peaks, $G_{in}$, and current valleys as a function of the band gap.

In summary, we have theoretically investigated the NDR in graphene symmetric DB RTDs and demonstrated an almost structure-free and back gate-controlled lowest OW. This remarkable phenomenon stems from the ambipolar transport in graphene and may be applied in OW-dominated NDR devices. We have also found that, appropriate structural parameters are necessary for the NDR feature and a tunable band gap can enhance exponentially the PVR. The competition between hole-to-electron transport, Klein tunneling, and resonant tunneling is the main mechanism for such a NDR structure.

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