

Quantum Conductance Manipulation of Graphene Nanoribbon Field Effect Transistor

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Abstract—The quantum transport characteristics of the strained graphene nanoribbon nanodevice are investigated under the effect of both ac-field of different frequencies and magnetic field. This nanodevice is modeled as follows: A graphene nanoribbon is connected to two metallic leads. These two metallic leads operate as a source and a drain. The conducting substance is the gate electrode in this three-terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of graphene nanoribbon channel. The substances at the graphene nanoribbon/ metal contact are controlled by the back gate. The photon-assisted tunneling probability is deduced by solving the Dirac eigenvalue differential equation and the corresponding conductance is also, derived using Landauer-Buttiker formula. The band structure parameters of graphene nanoribbon as the energy gap, the C-C bond length, the hopping integral, Fermi energy and the width are modulated by uniaxial strain. Results show that the conduction mechanism through the nanodevice is enhanced by the interplay between the transport charge Dirac fermions and the photons energy of the induced ac-field. Also, according to the results obtained in the present paper that the electronic transport through the present investigated graphene nanoribbon field effect transistor occurs by variable range hopping. The present research is very important in the field nanotechnology, that is, the present graphene nanoribbon nanodevices could be applied as digital nanoelectronics, logic gates, information technology, spintronics and photodetectors.

Keywords— *graphene nanoribbon; nanodevice; field effect transistor; quantum conductance*

I. INTRODUCTION

The advances of nanoscience and nanotechnology have enabled new approaches to designing and controlling the properties of materials at the atomic and molecular length scales. Recently graphene, a two-dimensional (2D) sheet of sp^2 - bonded carbon honeycomb lattice, has been considered as a promising material for many advanced applications in future electronics, such as ballistic single-electron transistors and interconnects [1 - 3]. The high

electron/hole mobility in graphene is very promising for future electronics devices [4-7]. The 2D graphene sheet demonstrates a zero band gap. For practical applications in semiconductor technology, the band gap of graphene has to be tuned to a finite value. A series of strategies were explored to engineer the band gap of graphene, for example, by applying an external electric field [8-11] or utilizing multilayer graphene structures.[11,12] and by inducing external strain [13-18]. A band gap can be created by patterning the 2-D graphene into a nanometer-wide graphene nanoribbon (GNR); this has been predicted theoretically [19–21] and realized experimentally [22 – 24]. Due to quantum confinement, graphene nanoribbons can have band gap, depending on their width and orientation relative to the graphene crystal structure [25]. Unlike single walled carbon nanotubes (SWCNTs), which are mixtures of metallic and semiconducting materials, a recent experiment [24] demonstrated that all sub-10 nm GNRs are semiconducting due to the edge effects, which make them more attractive for electronic device applications. Depending on the nature of the nanoribbon edges, one gets two symmetry groups; armchair graphene nanoribbon (aGNR) and zigzag graphene nanoribbon (zGNR). Armchair and zigzag GNRs show metallic or semiconducting electronic properties [26] depending on the number of dimer rows, N along transverse direction. N is related to the width of the nanoribbon [27]. Electron dynamics of both graphene nanoribbons have different properties, mostly due to the Berry phase and pseudo-spin [28]. Edge states have significant contribution to graphene properties, because in a nano-meter size ribbon, massless Dirac fermions can reach the edges within a femto-second before encountering any lattice effects, and avoiding electron-electron interaction, electron-phonon interaction, etc.

The purpose of the present paper is to investigate the quantum transport characteristics of graphene nanoribbon field effect transistor under the influence of both the ac-field with different frequencies and magnetic field. The effect of an external strain on the quantum transport characteristics of graphene nanoribbons is taken into consideration.

II. THEORETICAL MODEL

In this section we shall derive an expression for the conductance, G , of graphene nanoribbon nanodevice under the effects of both ac-field with different

frequencies and magnetic field. This can be achieved by proposing the following model of graphene nanoribbon nanodevice as follows:

A graphene nanoribbon is connected to two metallic leads. These two metallic leads operate as a source and a drain. The conducting substance is the gate electrode in this three-terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of graphene nanoribbon channel. The substances at the graphene nanoribbon/ metal contact are controlled by the back gate. The Dirac fermion charge carrier tunneling through the present investigated nanodevice is induced by an external applied ac-field which is given by:

$$V = V_{ac} \cos \omega t \quad (1)$$

where V_{ac} is the amplitude of the applied ac-field and ω is its frequency. Using Landauer-Buttiker formula, the conductance, G , is given by [29-32]:

$$G(E) = \frac{4e^2}{h} \cdot \sin \delta \cdot \int_{E_F}^{E_F + n\hbar\omega} dE \cdot \Gamma_{withphotons}(E) \cdot \left(-\frac{\partial f_{FD}}{\partial E} \right) \quad (2)$$

where δ is the phase difference between the incident electrons, e is the electronic charge, h is the Planck's constant, $\Gamma_{withphotons}(E)$ is the photon-assisted tunneling probability, E is the energy of the tunneled electrons and $\left(-\frac{\partial f_{FD}}{\partial E} \right)$ is the first derivative of the Fermi-Dirac distribution function and it is expressed as:

$$\left(-\frac{\partial f_{FD}}{\partial E} \right) = (4k_B T)^{-1} \cdot \cosh^{-2} \left(\frac{E - E_F + n\hbar\omega}{k_B T} \right) \quad (3)$$

where E_F is the Fermi-energy, T is the absolute temperature and k_B is Boltzmann constant. We shall now derive an expression for the photo-assisted tunneling probability as follows:

The transport of quasiparticle Dirac fermions in graphene nanoribbon nanodevice is described by the following Dirac Hamiltonian, H_0 , which is given as [18,33]:

$$H_0 = -i \hbar v_f \sigma \nabla + V_b \quad (4)$$

Where v_f is the Fermi velocity, $\sigma = (\sigma_x, \sigma_y)$ are the Pauli matrices and V_b is the barrier height. Since the present graphene nanoribbon is connected to two metallic leads and applying a top gate with gate voltage, V_g , also the transport of quasiparticle Dirac fermions are influenced by applying both an ac-field and magnetic field. So, accordingly Eq.(4) can be rewritten as follows:

$$H = H_0 + eV_{sd} + eV_g + eV_{ac} \cos(\omega t) + \frac{\hbar e B}{2m^*} \quad (5)$$

where V_{sd} is the bias voltage, \hbar is the reduced Planck's constant and m^* is the effective mass of quasiparticle Dirac fermions in graphene nanoribbon. Now, due to transmission of these quasiparticles Dirac fermions through the present investigated nanodevice, a transition from central band to side-bands of graphene nanoribbon at energies equals $E \pm n\hbar\omega$ [18, 35,36], where n is an integer with values $0, \pm 1, \pm 2, \dots$. The Dirac eigenvalue differential equation is given by [34, 35]:

$$H \Psi = E \Psi \quad (6)$$

where E is the scattered energy of quasiparticle Dirac fermions. The solution of Eq.(6) gives the following eigenfunctions [18, 36]. The eigenfunction of incident quasiparticle Dirac fermions is:

$$\Psi_{in}(x, y; t) = \sum_{n=1}^{\infty} J_n \left(\frac{eV_{ac}}{n\hbar\omega} \right) \cdot \left[\begin{array}{l} \left[\begin{array}{l} 1 \\ s e^{i\phi} \end{array} \right] \cdot \exp(i(k_x x + k_y y)) + \\ \left[\begin{array}{l} 1 \\ -s e^{-i\phi} \end{array} \right] \cdot \exp(i(-k_x x + k_y y)) \end{array} \right] e^{-in\omega t} \quad (7)$$

The eigenfunction of the transmitted quasiparticle Dirac fermions is:

$$\Psi_{tr}(x, y; t) = \sum_{n=1}^{\infty} J_n \left(\frac{eV_{ac}}{n\hbar\omega} \right) \cdot \left[\begin{array}{l} t \left[\begin{array}{l} 1 \\ s e^{i\phi} \end{array} \right] \cdot \exp(i(k_x x + k_y y)) \end{array} \right] e^{-in\omega t} \quad (8)$$

Where r and t are the reflection and transmission amplitudes, $s = \text{sgn}(E)$ is signum function of E and ϕ is the angle of incidence of the quasiparticle Dirac fermions (see Eqs.7, 8). The wave vectors k_x and k_y are expressed in terms of ϕ as:

$$k_x = k_f \cos \phi \quad \text{and} \quad k_y = k_f \sin \phi \quad (9)$$

where k_f is the Fermi wave vector. It is well known that electrons will be laterally confined in narrow graphene nanoribbons, similar to constrictions in conventional 2DEGs. The narrow width yields the quantization of the wave vector in lateral direction: $k_y W \approx m' \pi$ (for $m' \geq 1$) where a square-well potential equal to the nanoribbon width (W) is presumed [26,37]. The wave vector k_y will have the following form:

$$k_y = \frac{m' \pi}{W} \quad (10)$$

The eigenfunction inside the region of the barrier is given by:

$$\Psi_b(x, y; t) = \sum_{n=1}^{\infty} J_n \left(\frac{eV_{ac}}{n\hbar\omega} \right) \cdot \left[\begin{array}{l} \left(\begin{array}{l} \alpha \\ s'\beta e^{i\theta} \end{array} \right) \cdot \exp(i(q_x x + k_y y)) + \\ \left(\begin{array}{l} \alpha \\ -s'\beta e^{-i\theta} \end{array} \right) \cdot \exp(i(-q_x x + k_y y)) \end{array} \right] e^{-in\omega t} \quad (11)$$

where $s' = \text{sgn}(E - V_b)$ & $\theta = \tan^{-1}(k_y / q_x)$ and $q_x = (k_f'^2 - k_y^2)^{1/2}$. The wave vector k_f' is given by:

$$k_f' = \sqrt{\frac{(V_b - E')^2 - \left(\frac{E_g}{2}\right)^2}{(\hbar v_f)^2}} \quad (12)$$

where E_g is the energy gap and the parameter E' is expressed as:

$$E' = E - eV_{sd} - eV_g - V_b - n\hbar\omega + \frac{\hbar eB}{2m^*} \quad (13)$$

In Eqs. (7, 8, 11), J_n is the n th order Bessel function. This solution must be generated by the presence of different side-bands, n , which come with phase factors $\exp(-i n \omega t)$ that shifts the center energy of the transmitted quasiparticle Dirac fermions by integer multiples of $\hbar\omega$ [38]. The parameters α and β in Eq.(11) are given by:

$$\alpha = \sqrt{1 + \frac{s' \left(\frac{E_g}{2\hbar v_f} \right)}{\sqrt{\left(\frac{E_g}{2\hbar v_f} \right)^2 + k_f'^2}}} \quad (14)$$

and

$$\beta = \sqrt{1 - \frac{s' \left(\frac{E_g}{2\hbar v_f} \right)}{\sqrt{\left(\frac{E_g}{2\hbar v_f} \right)^2 + k_f'^2}}} \quad (15)$$

The parameters α & β are corresponds to K-point and K' - point respectively. Now, applying the boundary conditions Eqs. (7, 8, 11) at the boundaries of the barrier, we get the tunneling probability, $\Gamma_{withphotons}(E)$ as follows:

$$\Gamma_{withphotons}(E) = \sum_{n=1}^{\infty} J_n^2 \left(\frac{eV_{ac}}{n\hbar\omega} \right) \cdot \left| \frac{1}{\cos(q_x d) - i(ss'\eta \cdot \sec(\phi)\sec(\theta) + \tan(\phi)\tan(\theta)) \cdot \sin(q_x d)} \right|^2 \quad (16)$$

where d is the barrier width. The parameter η is given as:

$$\eta = \frac{\sqrt{\frac{E_g^2}{4(\hbar v_f)^2} + k_f'^2}}{k_f'} \quad (17)$$

Substituting Eq.(16) into Eq.(2) and the complete equation for the conductance, G , will be solved numerically as it will be shown in the next section. Since we want to compute the conductance of the present nanodevice under the influence of strain, then the band gap of both armchair and zigzag graphene nanoribbons varies with strain as follows:

The relation between the energy gap of the armchair graphene nanoribbons and the external strain [39] is given by as:

$$E_g = 2 \left| \gamma_1 + 2\gamma_2 \cos\left(\frac{p\pi}{N+1}\right) \right| \quad (18)$$

where γ_1 and γ_2 are the strained hopping parameters, p is an integer and N is the number of dimer lines across the ribbons. The strained hopping parameters γ_1 and γ_2 are related to the unstrained hopping parameter, γ_0 , by the following equations as [39]:

$$\gamma_1 = \frac{\gamma_0}{(1+\varepsilon)^2} \quad \text{and} \quad \gamma_2 = \frac{\gamma_0}{\left(1 + \frac{\varepsilon}{4}\right)} \quad (19)$$

where ε is the uniaxial strain. Also, the relation between the energy gap, E_g , of the zigzag graphene nanoribbon and the strain, ε , is given by [40]:

$$E_g = 3\gamma_0 S_t (1 + \nu_z) \varepsilon \quad (20)$$

where S_t is constant and its value is 1.29 [40] and ν_z is Poisson's ratio and its value is 0.16. The variation of the effective mass, m^* , of the quasiparticle Dirac fermion with the energy gap of the graphene nanoribbon is given by [41]:

$$m^* = \frac{2\hbar^2}{9\gamma_0^2 a^2} \cdot E_g \quad (21)$$

where a is the equilibrium bond length of the graphene nanoribbon.

III. RESULTS AND DISCUSSION

Numerical calculations are performed for both strained armchair and zigzag graphene nanoribbons with certain widths. This can be achieved by computing the conductance, G , (see Eq.2) under the

effects of the induced ac-field with different values of frequency in the range of infrared and also the effect of applied magnetic field. The following values are: the barrier height, V_b , equals 0.12 eV and its width $d=10\text{nm}$, the unstrained nearest neighbor hopping parameter, γ_0 equals 2.7 eV, the unstrained C-C bond length equals 0.142 nm, and the angle of incidence of the quasiparticle Dirac fermions, ϕ , equals 1.335 rad [18, 21]. The unstrained Fermi-energy, E_F , is determined in terms of γ_0 through the following equation $E_F = 0.072 \gamma_0$ [2, 42]. It must be noted that the hopping integral γ_0 between the π orbitals of armchair graphene nanoribbon (AGNR) is altered upon strain. This causes the up and down shift, the σ' band, to the Fermi level, E_F [42]. The strained hopping integral, γ' is related to the unstrained hopping integral, γ_0 , through the following equation [43, 44]:

$$\gamma' = \gamma_0 \left(\frac{a}{a'} \right)^2 \quad (22)$$

where a is the unstrained C-C bond length, and a' is the strained C-C bond length. An armchair ribbon is cut so that the edge looks as if it consists of repeated armchairs [23, 42]. Each edge is terminated by atoms of the A- and B-sublattice. The strained width, W_a , of an armchair nanoribbon can be defined in terms of the number of dimer lines N_a :

$$W_a = (N_a - 1) \frac{\sqrt{3} a'}{2} \quad (23)$$

Also, for zigzag graphene nanoribbons (ZGNR), the atoms at one edge are of the same sublattice, e.g. A atoms at the left edge and B atoms at the right edge. The strained width, W_z , of a zigzag nanoribbon is now identified with the number of zigzag chains N_z , as [23, 42]:

$$W_z = (N_z - 1) \frac{3a'}{2} \quad (24)$$

Now, the effect of uniaxial strain is modeled as a modification to the tight-binding nearest neighbor hopping integral (see Eq.22) and the corresponding strained C-C bond length, a' , and the corresponding widths, W_a and W_z (see Eqs.23, 24) in order to give an optimum values [45]. Also, by applying moderate uniaxial strain, ($\varepsilon = 15\%$), in order to estimate the energy band gaps of both armchair and zigzag graphene nanoribbons (see Eqs. 18, 20) and the effective mass, m^* (see Eq.21) . The calculations are performed to simulate the equations (18, &20) and using the density functional theory [45].

The features of the results for the conductance, G , (see Eq. 2) for both armchair and zigzag graphene nanoribbons (GNR) are:

-Fig.(1) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the frequencies of the induced ac-field for armchair GNR.

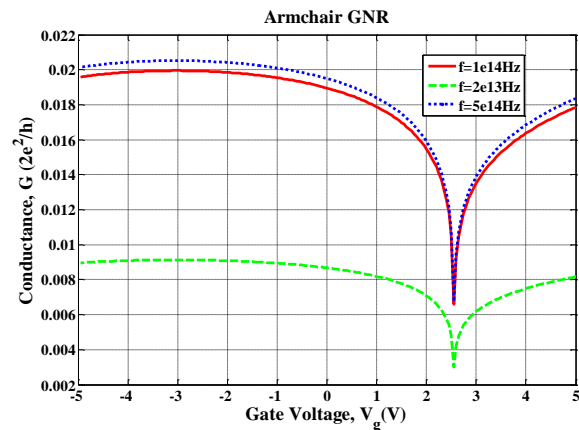


Fig. 1 The variation of the conductance, G , with the gate voltage, V_g , at different frequencies (Armchair GNR).

-Fig.(2) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the frequencies of the induced ac-field for zigzag GNR.

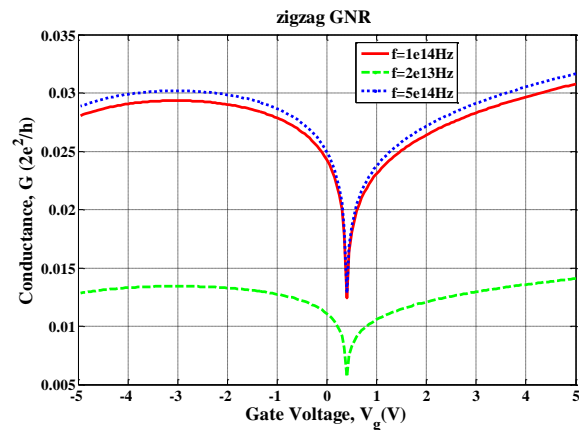


Fig. 2 The variation of the conductance, G , with the gate voltage, V_g , at different frequencies (zigzag GNR).

As shown from figs. (1, 2) both for armchair and zigzag graphene nanoribbons that the conductance, G , decreases as the gate voltage, V_g , increase in the negative region of V_g , until it attains a minimum value for positive value of V_g and then increases. The minimum values of the conductance, G , are:

For armchair graphene nanoribbons, $G_{\min}=0.006762$ at $V_g = 2.55$ V when the frequency of the induced ac-field equals 1×10^{14} & 5×10^{14} Hz. While for frequency is 2×10^{13} Hz,

$$G_{\min} = 0.003013 \text{ at } V_g = 2.55 \text{ V.}$$

For zigzag graphene nanoribbons, $G_{\min} = 0.01283$ at $V_g = 0.4$ V when the frequency of the induced ac-field equals 1×10^{14} & 5×10^{14} Hz. While for frequency is 2×10^{13} Hz,

$$G_{\min} = 0.005688 \text{ at } V_g = 0.4 \text{ V.}$$

It is well known that the effect of the induced ac-field on the transport through the present investigated graphene nanoribbon nanodevice might be achieved for those charge carriers with energy component, E ,

$E \pm \hbar\omega$, $E \pm 2\hbar\omega$,....., where $\hbar\omega$ is the photon energy of the induced ac-field [30 - 32, 46]. These energy components are called side-bands [45 - 48]. A positive value is due to the absorption of photons and negative value is due the emission of photons during the tunnel process. The interplay between the transport charge Dirac fermions and the induced photons increases strongly as the energy of these photons increases (see Figs. 1, 2). As a consequence, this interplay affects the side-bands and the tunneling rates [30 - 32, 48- 50].

- Fig. (3) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the applied magnetic field, B for armchair GNR.

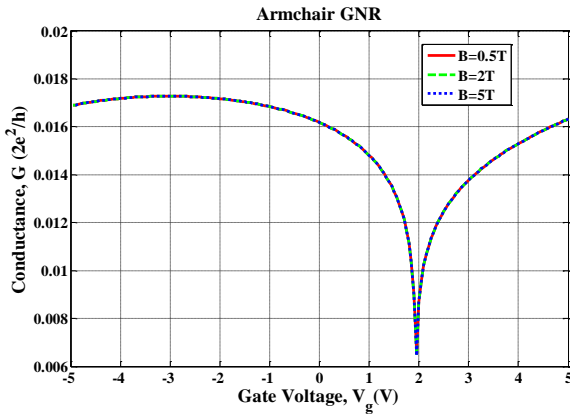


Fig. 3 The variation of the conductance, G , with the gate voltage, V_g , at different values of the magnetic field (Armchair GNR).

- Fig. (4) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the applied magnetic field, B for zigzag GNR.

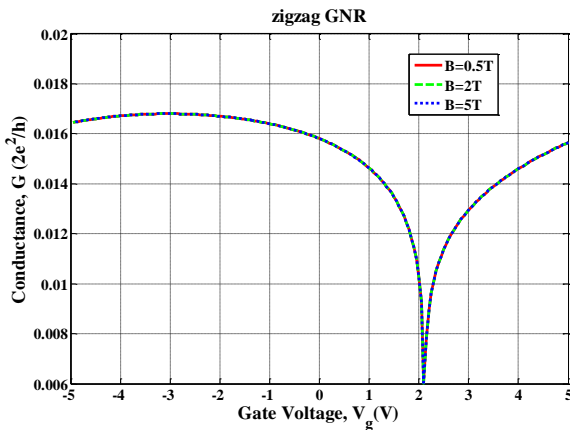


Fig. 4 The variation of the conductance, G , with the gate voltage, V_g , at different values of the magnetic field (zigzag GNR).

As shown from figs. (3, 4) both for armchair and zigzag graphene nanoribbons that the conductance, G , decreases as the gate voltage, V_g , increase in the negative region of V_g , until it attains a minimum value for positive value of V_g and then increases. The minimum values of the conductance, G , are:

- For armchair graphene nanoribbon, $G_{\min} = 0.006529$ at $V_g = 1.95$ V for all values of the applied magnetic field, B , (0.5 T, 2T, 5T).

- For zigzag graphene nanoribbon, $G_{\min} = 0.006058$ at $V_g = 2.1$ V for all values of the applied magnetic field, B , (0.5T, 2T, 5T).

- Fig. (5) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the temperature, T for armchair GNR.

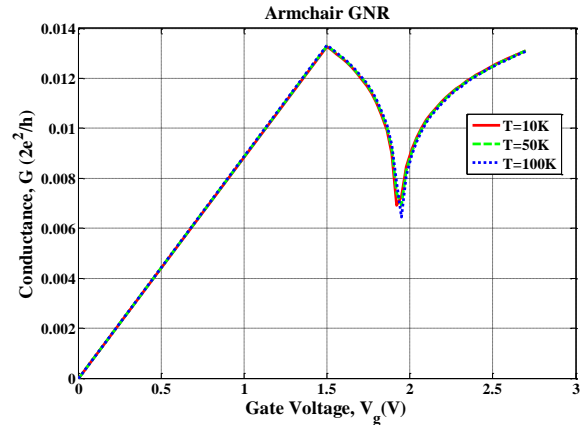


Fig. 5 The variation of the conductance, G , with the gate voltage, V_g , at different values of the temperature (armchair GNR).

- Fig. (6) shows the variation of the conductance, G , with the gate voltage, V_g , at different values of the temperature, T for zigzag GNR.

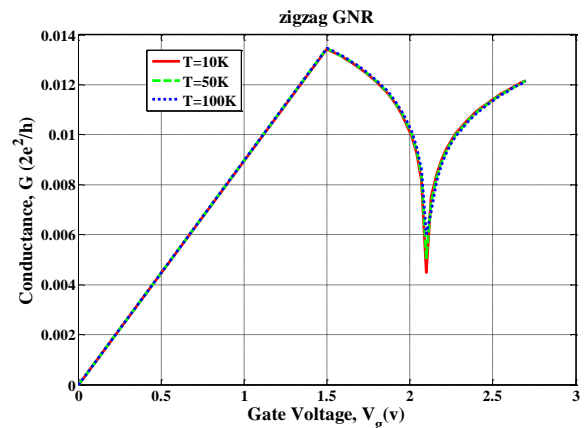


Fig. 6 The variation of the conductance, G , with the gate voltage, V_g , at different values of the temperature (zigzag GNR).

As shown from fig. (5) for armchair graphene nanoribbon that the conductance, G , varies linearly with the gate voltage, V_g , until it attains a maximum value $G_{\max} = 0.001331$ at $V_g = 1.5$ V and then it decreases until it attains a minimum value $G_{\min} = 0.006905$ at $V_g = 1.92$ V (temperature $T = 10$ K), and the same minimum value of the conductance at $V_g = 1.95$ V (temperature $T = 50$ K). While the conductance, G , attains a minimum value equals 0.006457 at $V_g = 1.95$ V (temperature $T = 100$ K). Also for zigzag graphene nanoribbon, the same trend for the variation of the conductance with the gate voltage and the data are the following: $G_{\max} = 0.01347$ at $V_g = 1.5$ V for all temperatures considered (see Fig.(6)). While the minimum values of the conductance, G , at $V_g = 2.1$ V are, respectively, 0.00603 ($T = 10$ K), 0.005072 ($T = 50$ K) and 0.004475 ($T = 100$ K). These results for both

armchair and zigzag graphene nanoribbons (see figs. 5, 6) are found in concordance with those in the literature [51, 52]. After the minimum values of the conductance for both armchair and zigzag graphene nanoribbons, we notice the increase of the conductance with the gate voltage (see Figs 5, 6). It is known that, due to quantum confinement effects, AGNRs can be classified into three families according to the width of the AGNR in which the number of C atoms in the zigzag direction falling in the categories of $3p$, $3p+1$, and $3p+2$, where p is a positive integer [20, 21]. In the present paper we consider the case $3p+1$ where $p = 12$ and the strained width, W_a , for the present investigated armchair graphene nanoribbon is computed and it has value equals 5.091 nm. Also, the computed value of the strained width, W_z , for the zigzag graphene nanoribbon is 6.647 nm ($N_z = 28$) [26]. The realization of electronic devices such as field-effect transistors will require controlling and even switching off the electrical conductance by means of gate electrodes, that is, conduction can be switched off by tuning the band gap by external strain [18, 22]. So, according to the variation of the conductance, G , with the gate voltage, V_g , (see figs.1 - 6), we might expect that the conduction can be switched off by the present investigated graphene nanoribbon field effect transistor.

Also, when electrons are strongly localized, they can hop from one electron state to another yielding an electric current. In general, two hopping mechanisms are distinguished: nearest neighbor hopping and variable range hopping [53]. Since the present results for the variation of the conductance with the gate voltage are performed at low temperatures, T , (see figs. 5, 6) within the range T equals 10, 50, 100 K. Then the electronic transport through the present investigated graphene nanoribbon field effect transistor occurs by variable range hopping [54]. The present results are found in concordance with those results in the literature [16, 55].

IV. CONCLUSION

The quantum transport characteristics of both armchair and zigzag graphene nanoribbons field effect transistor are investigated in the present paper under the effects of the induced ac-field with different frequencies and magnetic field. The effect of uniaxial strain is taken into consideration. The conductance is derived using Landauer-Buttiker formula. The interplay between the transports charges Dirac fermions and the induced photons increases strongly as the energy of these photons increases. As a consequence of this interplay, that is, this interplay affects on the sidebands and the tunneling rates. Results show that the present armchair graphene nanoribbon nanodevice might be used for digital nanoelectronics and logic gates. Also, zigzag graphene nanoribbon nanodevice could be used for information technology, spintronics and photodetectors.

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