Negative differential conductance and effective electron mass in highly asymmetric ballistic bilayer graphene nanoribbon

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ABSTRACT

We present a simplified theory of the effective momentum mass (EMM) and ballistic current–voltage relationship in a degenerate two-folded highly asymmetric bilayer graphene nanoribbon. With an increase in the gap, the density-of-states in the lower set of subbands increases more than that of the upper set. This results in a phenomenological population inversion of carriers, which is reflected through a net negative differential conductance (NDC). It is found that with the increase of the ribbon width, the NDC also increases. The population inversion also signatures negative values of EMM above a certain ribbon-width for the lower set of subbands, which increases in a step-like manner with the applied longitudinal static bias. The well-known result for symmetric conditions has been obtained as a special case.

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The high Fermi velocity of electrons in bilayer graphene (BG) has recently found potential applications in the realm of mesoscopic devices and in certain aspects of particle physics that are achievable in tabletop experiments [1]. The first principle studies [2] and tight-binding model [3] applied on BG by incorporating all important interlayer interactions show that the conduction and valance bands slightly overlap near the Fermi level. These outcomes exhibit that BG should be a semimetallic material rather than a zero band gap material. A BG can also be tuned near the Dirac-point between two degenerate conduction and valance bands. This band gap tuning can be externally controlled by applying either a transverse electric field [4] or by selective doping depending whether the difference is zero or non-zero respectively.

For investigating two port carrier transport properties, the selective doping technique is mainly preferred, since in such cases, there is no need of a transverse electric field. Whether the carrier transport in BG, or in any other material, is diffusive or ballistic at a certain temperature, is completely determined by the carrier’s mean free path (MFP) length at that temperature. Ballistic transport is said to occur when this length becomes greater than the material dimension. Otherwise it is called diffusive transport. In the past few years, investigations on both the ballistic and diffusive transport properties of carriers in BG have been done for their possible applications in nanoelectronics, spanning from the transistors to long interconnects in ultra-small integrated systems [6–15]. Extensive analyses of Hwang and Das Sarma [16] and Kubakaddi [17] suggest that although BG has an extremely nonlinear band structure, the overlap integral can be avoided since the Coulomb potential does not play a role in the determination of the phonon matrix element. Their arguments fit well in explaining electron mobility at room temperature in BG which is about 10^5 cm^2 V^−1 s^−1. Their results can also be experimentally realized [18,19].

One such transport property is the carrier effective mass which is strongly connected to carrier mobility and is known to be one of the most important physical quantities used in the analysis of semiconductor devices under different physical conditions [20]. Although there are various definitions of the effective electron mass [21], it is the effective momentum mass (EMM) that should be regarded as the basic quantity [22] for the description of the carrier transport of the conduction band electrons with arbitrary band non-parabolicity [23]. However, with increasing band non-parabolicity, the EMM becomes a function of electron energy. Under carrier degeneracy, only the electrons at the Fermi surface participate in the conduction process, and hence the investigation of the EMM corresponding to the Fermi level is of interest. It may also be noted that the Fermi energy is, in turn, determined by the carrier dispersion relation and degeneracy, and thus these two features explain the behavior of the EMM in degenerate materials.

In a BG sheet, carriers are confined in a 2D plane. A further structural confinement along the lateral direction transforms the 2D system to a 1D system resulting in BG nanoribbon (BGN). Recent fabrication method sono-chemically cuts chemically derived...
of tight binding (TB) formalism. We also report the ballistic
highly asymmetric BGN has yet to be investigated in the presence
of energy eigenvalues. When a longitudi-
the width of the BG is few nanometers, the resulting lateral car-
which may lead to a better thermoelectric material. In case, if
than those of corresponding single-walled carbon nanotubes[26]
providing a substantially lower resistance than copper wire having
unity aspect ratio [12]. Further, the ballistic electron thermal con-
ductance per unit width of graphene nano-ribbons can be smaller
layer of graphene has totally
relation which signatures a phenomenological negative differential
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Nevertheless, it appears from the literature that the EMM for a
highly asymmetric BGN has yet to be investigated in the presence
of carrier degeneracy. In this Letter, we present a simplified theo-
retical formulation of the EMM and a ballistic two port current-
fluence relationship in an asymmetric BGN within the framework
of tight binding (TB) formalism. We also report the ballistic I–V
relation which signatures a phenomenological negative differential
conductance (NDC) effect by considering the incorporation of the
subbands due to the splitting of both sets of conduction bands.

We start with the use of TB theory by assuming each mono-
layer of graphene has totally $l_y$ zigzag chains with $l_x$ atomic sites
on each chain for an asymmetric BGN sheet [8]. This leads to the
electron Hamiltonian near the K point as [4,8]
\[
H = \begin{pmatrix}
-\Delta/2 & 0 & 0 & \pi^\dagger \\
0 & \Delta/2 & 0 & \pi \\
0 & \pi^\dagger & -\Delta/2 & \gamma \\
\pi & 0 & \gamma & -\Delta/2
\end{pmatrix}
\]  
(1)
in which $l_y$ and $l_x$ are the width and length of the BG, $\Delta = \phi_1 - \phi_2$, $\phi_i$'s are the onsite potentials on each monolayer, $\pi\equiv v_F \hbar (-i\frac{\partial}{\partial x} + \frac{\pi}{\hbar})$ is the Berry phase momentum operator [4], $v_F$ is the Fermi velocity and $\gamma$ is the interlayer coupling constant. Modeling the BG as a two-coupled hexagonal lattice with a stacking pair of A–B type, the use of Eq. (1) and a Bloch-type eigen-
states $\psi(x, y) = (\psi_A, \psi_B, \psi_A^*, \psi_B^*)$, where, $\psi_i(x, y) = \phi_i(y)e^{ik_x x}$, in which, $i = A, B, A', B'$ leads to the following equations:
\[
-\nu_F \hbar \frac{\partial}{\partial y} - k_x \phi_B = \left( E + \Delta \right) \phi_A \\
\nu_F \hbar \frac{\partial}{\partial y} + k_x \phi_A = \left( E - \Delta \right) \phi_B \\
-\nu_F \hbar \frac{\partial}{\partial y} - k_x \phi_B^* = \left( E - \Delta \right) \phi_A^* - \gamma \phi_B \\
\nu_F \hbar \frac{\partial}{\partial y} + k_x \phi_A = \left( E + \Delta \right) \phi_B - \gamma \phi_A^*
\]  
(2)
in which $E$ is the electron energy as measured from the bottom
of the conduction band in a vertically upward direction. Taking the
values of $\phi_B$ and $\phi_A$ from Eqs. (3) and (2) and substituting them
in Eqs. (4) and (5) respectively, results in
\[
\left( k_x^2 - \frac{\partial^2}{\partial y^2} \right) \phi_A + \gamma E - \Delta/2 \left( \nu_F \hbar \right)^2 \phi_B = 0
\]  
(6)
and
\[
y' + \frac{E - \Delta/2}{(v_F \hbar)^2} \phi_A' + \left[ \left( k_x^2 - \frac{\partial^2}{\partial y^2} \right) - \left( E - \Delta/2 \right) \frac{(\nu_F \hbar)^2}{\gamma} \phi_B = 0\right.
\]  
(7)
Assuming the potentials to be constants, the solution is given by
\[
k^2 - \left( E - \Delta/2 \right) \frac{\gamma}{(v_F \hbar)^2} = \left( E + \Delta/2 \right) \frac{\gamma}{(v_F \hbar)^2}
\]  
(8)
in which, $k^2 = k_x^2 + k_y^2$. For a symmetric case ($\Delta = \phi_1 - \phi_2 = 0$), Eq. (8) becomes
\[
k^2 - \left( E - \Delta/2 \frac{\gamma}{(v_F \hbar)^2} \right) = \pm \gamma \left( E - \Delta/2 \frac{\gamma}{(v_F \hbar)^2} \right)^2
\]  
(9)
which at $k = 0$ converges to either $E = 0$ or $E = \pm \gamma$ for both $E > 0$
and $E < 0$ energy bands. This convergence is in accordance with
the well-known result [27] and proves the mathematical compati-
bility of our theory.

For an asymmetric BGN, we invoke the van Hove singularity condition $k_y = \frac{n_y \pi}{l_y}$ for the Bloch type wavefunction along the
y direction, which results in
\[
k^2_x + \left( \frac{\gamma}{(v_F \hbar)^2} \right) = \gamma \left( E - \Delta/2 \frac{\gamma}{(v_F \hbar)^2} \right)^2
\]  
(10)
in which, $n_y = 1, 2, 3, \ldots$ are the van Hove singularity quantum
numbers along the $y$ direction respectively. It readily appears that
Eqs. (8) and (10) generate two sets of degenerate subbands namely $E_+^\pm$, $E_-^\pm$, $E_+^\mp$ and $E_-^-$. Fig. 1 exhibits the energy spectrum for an
asymmetric BGN considering the lower conduction ($E_+^+$) and higher
valence band ($E_-^-$). The constant energy surfaces are the circles in the $k_x$–$k_y$ plane. With an increase in asymmetry, the gap opens as shown in Fig. 2. For an asymmetric BGN, Eq. (10) transforms to
\[
k_{x_\pm} = \frac{1}{\nu_F \hbar} \left[ E^2 + \Delta^2/4 - \left( \frac{n_y \pi \nu_F \hbar}{l_y} \right)^2 \right]^{1/2}
\]  
(11)
Fig. 3(b) exhibits the energy subband structure of an asymmetric
BGN. It appears that there is no inter-mixing of the conduction

\[
E_\pm = \Delta/2 \left( \frac{\gamma}{(v_F \hbar)^2} \right)^{1/2} \left( k_x^2 - \frac{\partial^2}{\partial y^2} \right)^{1/2} \phi_B = 0
\]  
(7)
energy subbands because of both $E^+$ and $E^-$. Also for $l_y = 5$ nm, there is a considerable opening of the gap about the zero level.

Using Eq. (3) and the spin and valley degeneracies ($g_s = g_v = 2$) [28], the density of states in an asymmetric BGN for both the upper (+) and lower (−) set of subbands can be derived as

$$N_{1D}^{\pm} = \frac{g_s g_v}{\pi \hbar v_F} \sum_{n_y=1}^{n_{max}} \left\{ E \pm \frac{E(y^2 + \Delta^2/2)}{E^2(y^2 + \Delta^2) - \frac{y^2\Delta^2}{4}} \right\}$$

$$\times \left[ E^2 + \frac{\Delta^2}{4} \left( \frac{n_y \pi \hbar v_F}{l_y} \right)^2 \right]^{-1/2} \left( H(E - E_{n_y}^\pm) \right)$$

(12)

in which $H$ is the Heaviside step function and the subband energies are given by the condition $k^2 = 0$, in which $E$ is replaced by $E_{n_y}^\pm$.

For a highly asymmetric case ($\Delta = \gamma$), Eqs. (11) and (12) reduce to

$$k^2 = \frac{1}{\hbar v_F} \left[ E^2 + \frac{\gamma^2}{4} - \left( \frac{n_y \pi \hbar v_F}{l_y} \right)^2 \right] \pm \sqrt{2E^2\gamma^2 - \frac{\gamma^4}{4}}^{1/2}$$

(13)

and

$$N_{1D}^{\pm}(E) = \frac{g_s g_v}{\pi \hbar v_F} \sum_{n_y=1}^{n_{max}} \left\{ E \pm \frac{E\gamma}{\sqrt{2E^2 - \frac{\gamma^2}{4}}} \right\}$$

$$\times \left[ E^2 + \frac{\gamma^2}{4} - \left( \frac{n_y \pi \hbar v_F}{l_y} \right)^2 \right]^{-1/2} \left( H(E - E_{n_y}^\pm) \right)$$

(14)

Fig. 3 exhibits the energy dispersion curve of a BGN. On comparing Figs. 2 and 3, it appears that the presence of quantization along the lateral direction smoothens the bulging nature of the $E^\pm$ subbands. We also see from Fig. 3(b) that the presence of the van Hove singularity has a striking effect on the energy subband structure of an asymmetric BGN. This is reflected in the fact that with an increase in $\Delta$, the lower set of subband energies starts decreasing in magnitude rather than increasing. This is directly opposite in nature to the $E^+$ conduction band as shown in Fig. 2. Also, it appears that with decreasing $\Delta$, the energy difference between the alternate subbands of both the lower and upper set diminishes.

Fig. 4 also signatures this fact. For both symmetric and asymmetric systems, the presence of $\gamma$ and $\Delta$ has a profound effect on the density-of-states function in a BGN. From Fig. 4, it appears that for a symmetric BGN, states are more available in the $E^+$ rather than the $E^+$ subband; however, with the opening of the gap, states...
in the $E_{\pm}^1$ subband increase. In this Letter, we report this phe-
omenological population inversion in an asymmetric BGN, which
may find remarkable applications in the area of optical electronics
and NDC systems.

From Fig. 2, we see that in BG, a change in $\Delta$ does not appreci-
cably change the magnitude of $E_{\pm}^1$ subband energies at $k = 0$ as
compared to that of $E_{\pm}^1$ energies. However, a lateral confinement
for e.g., of 5 nm, opens a gap of about 0.2 eV about the 0 energy
line at $k = 0$. It may be noted that due to the presence of two con-
duction bands in a BG, an extremely large transmission coefficient
for a highly asymmetric diffusive BGN might be achieved when the
carriers are transferred from the source to the drain. This is due to
the splitting of both the conduction energy bands into a number
of subbands.

Using Eq. (14), the carrier concentration can for this present
case be written as

$$n_{1D} = \int_{E_y}^{\infty} N_{1D}(E)f(E)\,dE + \int_{E_{\Delta y}}^{\infty} N_{1D}(E)f(E)\,dE$$

where $f(E)$ is the Fermi–Dirac occupation probability factor. The
bottom of the subband energies for the highly asymmetric case
are $E_{\pm}^1 = \pm (\Delta/2)[\pm (n_y) \pm \sqrt{(\Delta^2/4) - 4E_{\Delta y}(n_y)}/2]$. [22,23]

$$\left. d_{\pm}(n_y) = \frac{1}{\sqrt{2}} \left[ (\pm 1) \mp \frac{\gamma}{\sqrt{2}} \right] \right) \gamma \theta^2(n_y)$$

where $E_{\Delta y}(n_y) = \pm \sqrt{(\Delta^2/4) - 4E_{\Delta y}(n_y)}$.

Eq. (15) results in

$$n_{1D} = n_{1D}^0 + n_{1D}^1$$

in which, $n_{1D}^0 = \frac{2}{\pi} \int_{E_y}^{\infty} \sum_{n_y=-\infty}^{\infty} \frac{e^{i\pi n_y}}{(E_{\Delta y} - E_y)^2}$

$$\left. \left( \frac{E_y - E_{\Delta y}}{E_{\Delta y} - E_y} \right)^2 \times \frac{e^{-i\pi n_y}}{E_y} \right) \left[ \frac{\gamma}{\sqrt{2}} \right] \gamma \theta^2(n_y) \right) \gamma \theta^2(n_y)$$

$\theta^2(n_y) = \gamma \left( \frac{\gamma}{\sqrt{2}} \right) \gamma \theta^2(n_y)$

$\left. d_{\pm}(n_y) = \frac{1}{\sqrt{2}} \left[ (\pm 1) \mp \frac{\gamma}{\sqrt{2}} \right] \right) \gamma \theta^2(n_y)$

$E_{\Delta y}(n_y) = \pm \sqrt{(\Delta^2/4) - 4E_{\Delta y}(n_y)}$

where $\gamma = 0.4$ eV. [27] This has been exhibited in Fig. 5. For a heavily doped symmetric BGN, $E_F \gg \gamma$

$$m_{1D}^\Delta(E_F) = \frac{E_F}{v_F^2} \left( 1 + \frac{2\gamma}{\sqrt{2}E_F - \gamma^2} \right)$$

However, for a symmetric case,

$$m_{1D}^\Delta(E_F) = \frac{E_F}{v_F^2} \left( 1 + \frac{\gamma}{E_F} \right)$$

Eq. (19) exhibits the fact that the EMM in lower subband can
become negative if $E_F < \gamma$, where, $\gamma = 0.4$ eV [27]. This has been
exhibited in Fig. 5. For a heavily doped symmetric BGN, $E_F \gg \gamma$

$$m_{1D}^\Delta(E_F) = \frac{E_F}{v_F^2} \left( 1 + \frac{\gamma}{E_F} \right)$$

Using Eqs. (13) and (17), the EMM in a highly asymmetrical
($\Delta = \gamma$) BGN along the longitudinal direction can be derived as

$$m_{1D}^\Delta(E_F) = \frac{E_F}{v_F^2} \left[ \frac{1}{\sqrt{2}} \right] \gamma \theta^2(n_y)$$

$\left. E_{\Delta y}(n_y) \left( \frac{\gamma}{\sqrt{2}} \right) \gamma \theta^2(n_y)$$

Using Eqs. (13) and (17), the EMM in a highly asymmetrical
($\Delta = \gamma$) BGN along the longitudinal direction can be derived as

$$m_{1D}^\Delta(E_F) = \frac{E_F}{v_F^2} \left[ \frac{1}{\sqrt{2}} \right] \gamma \theta^2(n_y)$$

$\left. E_{\Delta y}(n_y) \left( \frac{\gamma}{\sqrt{2}} \right) \gamma \theta^2(n_y)$$

Using Eqs. (13) and (17), the EMM in a highly asymmetrical
($\Delta = \gamma$) BGN along the longitudinal direction can be derived as
such a case, mobility to them. For the contributions to electron mobility in BGN can mainly be due to the electronic bands possess a lower EMM. Hence, when in the diffusive regime, the BG value still remains.

The appearance of humps in the curves of Fig. 6 is due to the redistribution of the electrons among the quantized energy levels when the size quantum number corresponding to the highest occupied subband.

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