Manipulating chiral transmission by gate geometry: switching in graphene with transmission gaps

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We explore the chiral transmission of electrons across graphene heterojunctions for electronic switching using gate geometry alone. A sequence of gates is used to collimate and orthogonalize the chiral transmission lobes across multiple junctions, resulting in negligible overall current. The resistance of the device is enhanced by several orders of magnitude by biasing the gates into the bipolar npn doping regime, as the ON state in the near homogeneous nn−n regime remains highly conductive. The mobility is preserved because the switching involves a transmission gap instead of a structural band-gap that would reduce the number of available channels of conduction. Under certain conditions this transmission gap is highly gate tunable, allowing a subthermal turn-on that beats the Landauer bound on switching energy limiting present day digital electronics.

The intriguing possibilities of graphene derive from its exceptional electronic and material properties [1–3], in particular its photon-like bandstructure [4], ultrahigh mobility [5], pseudospin physics and improved 2-D electrostatics [6]. Its switching ability, however, is compromised by the lack of a band-gap [7], while opening a gap structurally kills the available modes for conduction, degrading mobility [7, 8]. This begs the question as to whether we can significantly modulate the conductivity of graphene without any structural distortion, thereby preserving its superior mobility and electron-hole symmetry. A way to do this is to open a transmission gap that simply redirects the electrons, without actually shutting off the density of states. The dual attributes that help graphene electrons in this regard are its photon like trajectories and chiral tunneling that makes the junction resistance strongly anisotropic, allowing redirection with gate geometry alone.

In an earlier paper, [9] we outlined how we can open a transmission gap by a tunnel barrier, angularly injecting the electrons with a quantum point contact (QPC) and then selectively eliminating the low incidence angle Klein tunneling [10] modes with a barrier, in that case a patterned antidot or an insulating molecular chain. When the critical angle for total internal reflection is lower than the angle subtended at the QPC by the barrier, electrons are unable to cross over across the junction. The result is a transmission gap that can be collapsed by driving the voltage gradient across the junction towards the homogenous pp or nn limit, creating a subthermal turn-on sharper than the Landauer binary switching limit of $kT ln 2$ for distinguishability ($kT ln 10$ for each decade rise in current). Beyond proof of concept, that geometry was limited by a paucity of QPC modes and the structural distortions near the barrier that create a larger effective footprint.

In this paper, we combine a split gated pn junction to collimate the transverse modes Fig. 1(a), with recently demonstrated [11,14] action of a tilted pn junction that increases the effective angle of incidence of the electrons. The conductance

Figure 1. (Color online) (a) Chiral tunneling in graphene manipulated with gate geometry, using two junctions tilted in opposite directions, (b) making their angle dependent transmission lobes orthogonal (left) and yielding negligible overall transmission for well separated gates (right). (c) The transmission gap creates a high ON-OFF at finite bias, $V_{DS} = 0.4V$ and room temperature. The ON current degrades slightly compared to homogeneous gapless graphene, but the OFF current is reduced by several orders of magnitude.
at zero temperature can be written as,

$$G(\varepsilon_F) = G_0 \sum_{n=1}^{M(\varepsilon_F)} T_n = G_0 M T_{av}$$  \hspace{1cm} (1)$$

where $G_0 = 2e^2/h$ is the conductance quantum for two spins, $M$ is the number of modes, $T_n$ is transmission of individual modes and $T_{av}$ is the average transmission over all modes. If all modes transmit with equal probability ($T$), the conductance can simply be written as $G_0 M T_{av}$. Due to the chiral nature of carriers in graphene, transmission in GPNJ is highly angle (mode) dependent making it necessary to work with the average transmission per mode $T_{av}$. Instead of eliminating the mode count $M$ as does a structural band-gap, we exploit instead the chiral tunneling that makes $T_{av}$ vanishingly small over a range of energy and controllable with geometry alone (Fig. 1). All modes are available for conduction in the ON state when the split gates are set to the same polarity and thus retaining high mobility of graphene.

**Engineering transmission gap with gate geometry.** Fig. 1 shows two $p n$ junctions tilted in opposite directions. Each junction exploits chiral tunneling that conserves pseudospin index and maximizes transmission at normal incidence (Klein tunneling), especially when they are smooth, i.e., the $p$ to $n$ transition occurs over a finite distance $2d$. A tilted junction rotates the transmission lobe accordingly, [11], shifting transmissions along opposite directions to make them orthogonal.

The mode-averaged transmissions across the dual junction can be decomposed as below (see appendix for details)

$$T_{av}(\theta) \approx \left[ \cos(\theta_L + \delta) \cos\theta_R \right]$$

$$\times \exp \left[ -\pi d \frac{k_{FL}k_{FR}}{k_{FL} + k_{FR}} \sin(\theta_L + \delta) \sin(\theta_R) \right]$$

$$\frac{1}{T_{eff}} \approx \frac{1}{T_1} + \frac{1}{T_2} - 1$$ \hspace{1cm} (2)

$$T_{av}(\varepsilon_F) = \frac{1}{2} \int T_{eff}(\theta) \cos\theta d\theta$$

$$= \left[ A \sqrt{k_F} e^{\pi k_F d \sin^2 \delta} \right]^{-1}$$ \hspace{1cm} (3)

which is vanishingly small for moderate doping (Fermi wavevector, $k_F = E_F/\hbar v_F$, $A$ is a constant, $A \approx 8$), gate split $2d$ and tilt angle $\delta$. The first equation arises from matching pseudospins across the junction, $L$ and $R$ denoting components to left and right of a junction (1,2) . The tilt angle $\delta$ modifies the incident angle by $\theta_L + \delta$ and the angle of refraction is related to incident angle through Snell’s law, $k_{FL} \sin(\theta_L + \delta) = k_{FR} \sin\theta_R$. The second equation assumes resistive addition of the junction resistances and ballistic flow in between. The mode count for an Ohmic contacted sample of width $W$ is given by $M = \frac{W}{k_F}$. The resulting total conductance $G_0 M T_{av}$ is negligible in the entire $p n$ junction regime, indicating that the transmission gap ($E_G$) exists if the carrier densities have opposite polarities,

$$E_G \approx V_0$$ \hspace{1cm} (4)
be extracted from
\[
I_{OFF} = G_0 \int_{\mu_0}^{\mu_s} M(E)T_{av}(E)dE
\approx G_0 M(E_F)T_{av}(E_F)V_{DS}
\]
(5)
convolved with the thermal broadening function at finite temperature. For uniformly doped graphene with ballistic transport,
\[
I_{ON} = G_0 M(E_F)V_{DS}
\]
(6)
so that the zero temperature ON-OFF ratio simply becomes,
\[
\frac{I_{ON}}{I_{OFF}} \approx |T_{av}(E_F)|^{-1} \sim A \sqrt{\kappa F d}(2e)^\pi k_F d \sin^2 \delta
\]
(7)
If the biasing is changed all the way from \textit{npn} to \textit{nnn}. Fig. 3(c, pink line) shows the change in dual tilted GPNJ current with gate voltage \(V_{G2}\) at room temperature and finite drain bias \(V_{DS}\), compared with a regular zero bandgap graphene based switch (black line). From the \textit{nn} to \textit{nnn} regime, we see little change in GPNJ current on a log scale. But towards the \textit{npn} regime, we see at least three orders of magnitude change when the Fermi window remains mostly within the transmission gap. Compared to the blue line, the ON current is reduced only slightly, while the OFF current is reduced by orders of magnitude. The reduction in ON current comes due to the fact that the doping is not quite uniform at the ON state across the \(n^+ n\) collimator (maintained at unequal doping to avoid a large voltage swing), whereupon the wave-function mismatch leads to lower current than usual. Fully ballistic transport assuming an Ohmic contacted high quality sample gives us an intrinsic ON current in the mA/\(\mu m\) regime. In this calculation the gate parameters are \(\delta_1 = |\delta_2| = \delta = 45^\circ\), \(d_1 = d_2 = 20\text{nm}\), \(V_{G1} = V_{G3} = +1\text{V}\), \(V_{DS} = 0.4\text{V}\).

Critical to the geometric switching is the prominence of angle-dependent chiral transmission across a tilted junction, especially in presence of charge puddles and edge reflection. Fig. 3 shows the mode averaged transmission extracted (see method in appendix) from the measured junction resistance for a single split junction, for varying tilt angles[14]. For an abrupt tilted junction \(T_{av} = 2/3\cos^4(\delta/2)\) in the symmetric \textit{pn} doping limit and represents an electronic analog of optical Malus’ law. The reduction in \(T_{av}\) happens due to the angular shift of transmission lobe (Fig. 1(b)) in low angular mode density region [11]. The numerically evaluated \(T_{av}\) generalized for a tilted split junction (solid lines) agrees with experimental data (dots) from all the devices. This angular dependence persists, for multiple diffusive samples [14]. The scaling of \(T_{av}\), in experiment thus confirms the angular shift of the transmission lobes and forms the basis of the proposed device. The data show a remarkable absence of specular edge scattering, and can be explained by the randomizing effect of roughness.

\[
\theta_C = \sin^{-1}\left|\frac{n_3}{n_2}\right| < \delta
\]
(8)
where \(n_3\) and \(n_2\) are doping concentrations on the two sides of junction 2. The resulting transmission vanishes over a range of energies (following from Eq. 8), which can be expressed as
\[
E_G = V_0 \frac{2 \sin \delta}{\cos^2 \delta}
\]
(9)
analogous to Ref. [9] despite being a different (simpler) geometry, with the tilt angle \(\delta\) replacing the barrier angle \(\theta_B\).

The tunability of the transmission gap for an abrupt junction bears a direct impact on the rate of change of current with gate voltage. For a semiconductor with fixed bandgap, this rate is \(k_B T \ln(10)/q\) and limits the energy dissipation in binary switching. The limit arises from the rate of change in overlap between the band-edge and the Fermi-Dirac distribution, normally set by the Boltzmann tail. In our geometry however, the transmission gap is created artificially with a gate bias \(V_0\) across the GPNJ, and can be collapsed by going from heterogeneous \(\textit{npn}\) towards the homogenous doping limit \(\textit{nnn}\). Such a collapsible transport gap will overlap with the Fermi distribution at a higher rate than usual with change in gate bias, leading to a subthermal switching steeper than the Lan-

**Figure 3.** (Color online) Benchmarking \(T_{av}\) with experiment [14] for a single tilted split junction for several doping conditions. Experiment shows good agreement with the theory confirming the scaling law of tilt, Eq. [A.5].
Figure 4. (Color online) Electron confinement in the proposed GPNJ device. Left: schematic of collimator-barrier pair that sequentially filters all propagating modes; middle column: band-diagrams showing bipolar OFF, \((n \delta n)\) vs unipolar ON, \((n^{-} n)\) states; (c) numerical current density plot from NEGF showing carrier reflections from the two junctions on top right (OFF), vs near uniform current flow at the bottom (ON). White (black) areas indicate high (low) local current density.

dauer limit. This results a lower gate voltage swing to turn on the device and thus reducing dissipation.

**Numerical simulation of quantum flow.** To demonstrate carrier trajectories in the proposed device, we numerically solve the Non-Equilibrium Green’s function Formalism (NEGF). The central quantity is the retarded Green’s function,

\[
G = (E I - H - U - \Sigma_1 - \Sigma_2)^{-1}
\]  

\(H\) is the Hamiltonian matrix of graphene, described here with a minimal one \(p_z\) orbital basis per carbon atom with \(t_0 = -3\text{eV}\) being the hopping parameter. \(\Sigma_{1,2}\) are the self energy matrices for the semi-infinite source and drain leads, assumed to be extensions of the graphene sheet (i.e., assuming excellent contacts) and \(\Gamma_{1,2}\) are the corresponding anti-Hermitian parts representing the energy level broadening associated with charge injection and removal. \(U\) is the device electrostatic potential. The current from \(i\)th atom to \(j\)th atom is calculated from

\[
I_{i,j} = \frac{2q}{h} \int dE \text{Im}[\bar{\varrho}^n_{i,j}(E)H_{j,i} - H_{i,j}\varrho^m_{j,i}(E)]
\]

where the electron correlation function, \(\varrho^m = \varrho \Sigma m \varrho^\dagger\) and in-scattering function, \(\Sigma^m = \Gamma S f_S + \Gamma D f_D\). The source and drain Fermi levels are at \(\mu_S = 0\) and \(\mu_D = -q V_{DS}\). To see the current distribution in the device, we apply a small drain bias \(V_{DS}\). \(I_{i,j}\) is nonzero only if the \(i\)th atom and \(j\)th atom are neighbors. The total current at an atomic site can be found by adding all the components, \(I_i = \sum_j I_{i,j}\).

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Appendix I

The average transmission per mode: Total transmission through a graphene heterojunction can be written as,

$$G(E_F) = G_0 \sum \frac{T(\theta)}{\Delta \theta} = \frac{k_F}{\Delta k_F} \int T(\theta) \cos \theta d\theta = G_0 M(E_F) \frac{1}{2} \int T(\theta) \cos \theta d\theta$$

Here we have used, angular spacing, $\Delta \theta = \Delta k_F/(k_F \cos \theta)$, mode spacing $\Delta k_F = 2\pi/W$ and number of modes, $M(E_F) = W k_F / \pi$. Comparing with Eq. 1, we can write,

$$T_{av}(E_F) = \frac{1}{2} \int T(\theta) \cos \theta d\theta$$

Transmission through a single $pn$ junction, where the potential changes smoothly from $p$ to $n$ over a distance $2d$ is given by,

$$T(\theta) = e^{-\pi k_F \sin \theta}$$

ignoring the wave-function prefactor, this is valid for moderate gate split distance $2d$. Let us consider the $T_{av}$ for a single split junction and a tilted junction separately.

$$G \approx G_0 M(E_F) \frac{1}{2} \int \frac{1}{\theta_0} d\theta e^{-\pi k_F d \theta^2}$$

$$= G_0 \left[ \frac{1}{2 \sqrt{k_F d}} \right]^M$$

(A.4)

$$T_{av} \approx \frac{1}{2 \sqrt{k_F d}}$$

with gate split. For an abrupt tilted junction,

$$G \approx G_0 \int \frac{\pi/2}{-\pi/2} T(\theta + \delta) d\theta$$

$$= G_0 \left[ \frac{2}{3 \cos \left( \frac{\delta}{2} \right)} \right]^M$$

(A.5)

due to reduced density of modes at the higher angular region, $T_{av} = \frac{1}{2} \cos^4 \left( \frac{\delta}{2} \right)$ is scaled with $\delta$. Therefore, a resistance measurement ($R_{Total} = 1/G$) will show an increase for a tilted device.

Transmission through dual tilt GPNJ device: In Fig. 2 we have two such junctions, each of them are tilted. Individual transmissions through the junctions becomes,

$$T_1(\theta) = e^{-\pi k_F \sin^2(\theta + \delta_1)}$$

$$T_2(\theta) = e^{-\pi k_F \sin^2(\theta - \delta_2)}$$

(A.6)

(A.7)

Since the tilt angle $\delta$ only modifies the angles of the incoming modes.

To get the total transmission, we combine the above two equations ignoring phase coherence to get the total transmission [16].

$$\frac{1 - T}{T} = \frac{1}{T_1} + \frac{1}{T_2} - 2 = e^{\pi k_F \sin^2(\theta + \delta_1)} + e^{\pi k_F \sin^2(\theta - \delta_2)} - 2$$

(A.8)

Overall transmission becomes

$$T(\theta) = \frac{1}{e^{\pi k_F \sin^2(\theta + \delta_1)} + e^{\pi k_F \sin^2(\theta - \delta_2)} - 1}$$

(A.9)

And

$$T_{av}(E_F) = \frac{1}{2} \int \frac{\pi/2}{-\pi/2} e^{\pi k_F \sin^2(\theta + \delta_1)} + e^{\pi k_F \sin^2(\theta - \delta_2)} - 1$$

$$T_{av}(E_F) \approx \frac{1}{8} \frac{1}{\sqrt{k_F d} e^{\pi k_F \sin^2 \delta}}$$

(A.10)

For $\delta_1 = \delta_2$.

Extracting $T_{av}$ from transport measurement: In the experiment [13], the junction resistance is extracted from

$$R_{expt} = |R(V_{G1}, V_{G2}) + R(V_{G2}, V_{G1}) - R(V_{G1}, V_{G1}) - R(V_{G2}, V_{G2})|/2.$$  

(A.11)

The above equation eliminates contact and device resistance due to scatterings and leaves out the resistance contribution from the $pn$ junction only. Theoretically the total resistance
$R_{Total} = 1/G$ can be divided into two parts (contact and device resistance). From Eq. 1,

$$R_{Total} = [G_0]^{-1} \frac{1}{MT_{av}}$$ (A.12)

$$= [G_0]^{-1} \left[ \frac{1}{M} + \frac{1 - T_{av}}{MT_{av}} \right]$$ (A.13)

In presence of a pn junction with non-unity $T_{av}$, the second term can be considered as the junction resistance,

$$R_j = [G_0]^{-1} \left[ \frac{1 - T_{av}}{MT_{av}} \right]$$ (A.14)

While the theoretical $T_{av}$ is already known (Eq. [A.5]), the experimental $T_{av}$ can be found by plugging the value of $R{j_{expt}}$ from measurement in Eq. [A.14]. The only unknown value remains is the number of modes at a particular gate voltage.

$$M = \frac{W}{\pi} \frac{\Delta E(V_G)}{\hbar V_F}$$ (A.15)

Here $\Delta E = \hbar V_F \sqrt{\frac{C_G V_G}{q}}$ is the shift of Dirac point with gate voltage $V_G$. The gate capacitance is calculated from a simple parallel plate capacitor model $C_G = \frac{t}{\epsilon_{ox}}$ where gate oxide thickness $t_{ox}$ is 100nm.