Current-voltage characteristics of graphene devices: interplay between Zener-Klein tunneling and defects

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We report a theoretical/experimental study of current-voltage characteristics (I-V) of graphene devices near the Dirac point. The I-V can be described by a power law \((I \propto V^\alpha, \text{with } 1 < \alpha \leq 1.5)\). The exponent is higher when the mobility is lower. This superlinear I-V is interpreted in terms of the interplay between Zener-Klein transport, that is tunneling between different energy bands, and defect scattering. Surprisingly, the Zener-Klein tunneling is made visible by the presence of defects.

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Zener tunneling\textsuperscript{1} is a concept known since the 30’s, which, in a solid, refers to the tunneling of carriers from one band to another through the forbidden energy gap (for example from the conduction to the valence band). This tunnel process is very intriguing in graphene because the energy gap is suppressed to zero and because of the peculiar charge carriers behaving as Dirac fermions \textsuperscript{2,3}. In particular, some of the carriers (those with the velocity parallel to the electric field) experience Zener tunneling without being backscattered \textsuperscript{4,5}, a behavior which is markedly different from the one in conventional semiconductors. The physics is the same as for relativistic electrons tunneling through a barrier, a phenomenon called Klein tunneling\textsuperscript{6} and, for this reason, we will use the term Zener-Klein (ZK) tunneling.

In view of the remarkable properties of ZK tunneling in graphene, it is understandable that an intensive endeavor was made to challenge it. So far, the effort was focused on graphene p-n junctions\textsuperscript{7–13}. In these devices, carriers tunnel through a sharp energy barrier induced with external local gate electrodes. Sophisticated nanofabrication techniques were employed to structure these local gates. For instance the insulator layer was very thin\textsuperscript{8,9,12}, the local gate was separated from the graphene by an air gap\textsuperscript{10,11}, or the local gate was extremely narrowed\textsuperscript{12}.

Here, we argue that Zener-Klein tunneling can be observed in graphene with the most common device layout (undoped, four-point configuration, and without any local gates) by simply measuring the I-V at room temperature. First, we provide an analytical semi-classical expression for the I-Vs as a function of the doping. In graphene, the ZK current manifests itself with a superlinear current \(I \propto V^\alpha\), with \(\alpha = 1.5\). Then, we study the role of defects with the “exact” (non-perturbative) non-equilibrium Green-function approach finding the counterintuitive result that charged impurities enhance the visibility of the ZK current. Finally, we report measurements showing that the I-Vs at the Dirac point is indeed described by power laws, \(I \propto V^\alpha\), with \(\alpha\) ranging from 1 to 1.4. The exponent \(\alpha\) is higher when the mobility is lower, consistently with our theoretical predictions.

In graphene ZK tunneling leads to unusual I-Vs as compared to those of semiconductors/insulators. Let us consider transport through a piece of a material and apply a voltage \(-V\) between the right (R) and left (L) sides. For a semiconductor with electronic gap \(E_g\), ZK tunneling is possible only for \(eV > E_g\), where \(e > 0\) is the electron charge (Fig. 1). On the contrary, in graphene (usually defined as a semi-metal) the gap is zero and, thus, ZK tunneling is possible for arbitrarily small \(V\).

More specifically, the two-dimensional electronic-band dispersion of graphene is a cone: \(\epsilon = \pm \hbar v_F \sqrt{k^2 + k^2}\perp\), where \(k (k\perp)\) is the wavevector-component parallel (perpendicular) to the current flow. During ballistic transport (in absence of scattering) \(k\perp\) is conserved. For a fixed \(k\perp\), the bands are hyperbolae with gap \(\Delta = 2\hbar v_F k\perp\) (Fig. 1). For any \(V\), there are conducting channels for which the tunneling is possible (with \(k\perp\) such that \(\Delta < V\)). We will show that this results in a tunneling current \(I \propto V^{3/2}\). By contrast, the ZK tunneling current in semiconductors vanishes exponentially at low \(V\).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{(Color online) Bands of the L and R contacts in a semiconductor and in graphene. The arrows represent the possible occurrence of Zener-Klein tunneling.}
\end{figure}

In graphene, within the Landauer approach, the current per unit of lateral length, \(J\), is

\[
J = \frac{4e}{\hbar} \int dk\perp \frac{1}{2\pi} \int_{-eV}^{eF} T(\epsilon, k\perp, V) d\epsilon = \frac{4e}{\hbar} \int_{-eV}^{eF} T(\epsilon, V) d\epsilon \tag{1}
\]

where the factor 4 accounts for spin and valley degeneracy and the transmission \(T(\epsilon, k\perp, V)\) is the probability that an electron (with energy \(\epsilon\) and perpendicular mo-
mentum $k_\perp$) is transmitted through the channel. We assume a uniform drop of the electrostatic potential along the current-flow direction, with constant electric field $V/l$, being $l$ the distance between the contacts.

![FIG. 2: (Color online) Electronic transport in graphene: theory. a: electronic bands of the left (L) and right (R) contacts. The hyperbolae are the bands corresponding to a finite $k_\perp$ (Δ = 2hνFk_\perp = 22 meV). In the L and R contacts the bands are filled up to $ε_F$ and $ε_F - ε_V$, respectively, where $ε_F > 0$ ($ε_F < 0$) corresponds to electron (hole) doping. b,c: electronic transmissions $T$ and $T$, defined as in Eq. 1 for $V = 0.1$ V and $l = 1$ μm. In the gray zone (the region corresponding to the Zener-Klein tunneling) $T$ and $T$ are magnified. b: ballistic case calculated with NEGF or with the WKB approximation. c: NEGF results in the ballistic case (no defects) or in the presence of long-range (lr) or short-range (sr) defects. d,e: calculated current $I$ per unit of lateral-length $l_W$ vs. $V$ (the voltage applied between the electrodes) as a function of the gate voltage ($V_g$). $V_g$ goes from 0 to 35 V with 5 V step, $l = 1$ μm. In the ballistic case (d), lines are approximated semi-classical results (i.e. the analytical curves from note 19), points are from the “exact” NEGF simulations.

The transmission can be calculated with the non equilibrium Green function (NEGF) method. To describe the purely ballistic case, we also use a semiclassical approach, based on the Wentzel-Kramers-Brillouin (WKB) approximation. The transmission $T^{WKB}(ε, k_\perp, V)$ can be equal to 1, 0, or to $T_{ZK} = \exp[-π(Δ^2/(4hνFV))]^{1.3}1$ (see the example in Fig. 2b). We call non-tunneling current (Fig. 2a), the one associated with carriers that always remain in the same band $π$ or $π^*$ ($T^{WKB} = 1$, light-shadowed (yellow) area in Fig. 2a). We call “Zener-Klein” current, the one associated with carriers that tunnel from the $π$ to the $π^*$ band ($T^{WKB} = T_{ZK}$, dark-shadowed (cyan) area in Fig. 2a). From Fig. 2b, the $T^{WKB}$ transmission is a good approximation to our most precise NEGF calculations.

In a graphene-based field-effect device, the density of the carriers $n$ can be varied by changing the gate voltage $V_g$, $n = V_gC_g/e$, being $C_g$ the gate-channel capacitance. Fig. 2b reports the current-voltage ($I$-$V$) curves in the ballistic regime obtained with the semiclassical WKB approach (by letting $T = T^{WKB}$ in Eq. 1) and with the “exact” NEGF method13, for various dopings (we use $C_g = 15 × 10^{-14}$ F/m$^2$118). The two methods give almost identical results (for the WKB case, we report in note 19 an analytical expression for the $I$-$V$ as a function of $ε_F$). For zero-doping ($V_g = 0$ V) there is no contribution from the non-tunneling current, the current is entirely due to ZK tunneling, and the $I$-$V$ curve is superlinear ($I \propto V^{3/2}$)102. As soon as the system is doped (already for $V_g = 5$ V) the ZK current is no more dominant (with respect to the non-tunneling current) and for small bias ($V < 0.1$ V) the $I$-$V$ is ohmic (linear).

Do we expect the superlinear ZK current to be visible in actual devices? At first sight the answer is no for two reasons. First, in actual devices, the carrier concentration is never exactly zero. Indeed it has been observed9 that the presence of charge impurities induces a spatial...
fluctuation of the Fermi level with respect to the Dirac point. As a result, it is difficult to achieve the experimental condition where ZK tunneling is observable (\(V_g=0\) in Fig. 2b). Second, the scattering of the carriers with optical phonons with energy \(\hbar \omega =0.15\) eV causes the current to saturate when increasing \(V\) to high values.\(^{18,20}\) This process occurs for \(eV > \hbar \omega /l_{el}\) (\(l_{el}\) is the carrier elastic scattering length, due to defects) and is, thus, particularly relevant for high-quality high-mobility samples (with high \(l_{el}\)). This saturation of the non-tunneling current induces a sublinearity \((I \propto V^\alpha\), with \(\alpha < 1\)) which tends to cancel the superlinearity \((\alpha > 1)\) of the ZK current, further masking it (see 17 for further discussion).

The situation is possibly changed by the presence of defects. Actual devices are characterized by defects which scatter electrons elastically (that is conserving the energy)\(^{18}\). Elastic defects can be neutral point defects or charged Coulomb impurities\(^{22}\) outside the graphene plane (usually at a distance \(\sim 1-2\) nm)\(^{23}\). Point defects affect the electrostatic potential seen by the carriers on a length scale smaller than the graphene unitary cell (short-range) and, thus, the carriers cannot be described in terms of electronic bands. On the other hand, charged impurities modify the potential uniformly on a length scale much longer than the unit cell (long-range) and the electronic bands are still a meaningful concept. The ZK current is expected to be more sensitive to short-range defects than to long-range ones. Indeed, the ZK current is determined by a transition between two bands whose relative energy is not affected by long-range defects. Moreover, long-range defects are expected to diminish the non-tunneling current. Overall, one could wonder whether the presence of long-range defects can be used to suppress the non-tunneling current and, thus, to make visible the ZK one.

To verify this hypothesis, we simulate disordered graphene within NEGF by considering both long- and short-range elastic defects.\(^{22}\) We remark that the NEGF approach provides an exact (non-perturbative) atomistic treatment of disorder. Defects are simulated by changing randomly the on-site potential by \(V_g = 0.1\) eV. This \(V_g\) is a realistic choice since it provides a low-bias conductivity in reasonable agreement with measurements.\(^{17}\)

From NEGF simulations, the presence of long-range defects diminishes the non-tunneling transmission (Fig. 2c) but, in general does not reduce the ZK one. For \(V=0.1\) V, long-range defects even increase the ZK transmission (Fig. 2c). We checked that short-range defects diminish, as expected, both the non-tunneling and the ZK transmission, with respect to the ballistic case (Fig. 2c). To see whether the relative increase of the ZK transmission with respect to the non-tunneling one can lead to measurable effects, in Fig. 2d, we show the theoretical \(I-V\) curves in the presence of long-range defects. The superlinear behavior (the signature of the ZK current) is still visible at \(V_g = 0\) (\(I \propto V^\alpha\), with \(\alpha = 1.4\) in Fig. 2c) and is also visible at finite \(V_g\).

We now turn our attention to measurements, carried out on single-layer graphene devices.\(^{24}\) Different devices were fabricated in a four-point configuration and have different mobilities \(\mu\) ranging from 80 to 20000 cm\(^2\)V\(^{-1}\)s\(^{-1}\) (low mobility corresponds to a higher density of defects).\(^{24}\) Fig. 3 shows a typical set of \(I-V\) characteristics for different \(V_g\) applied on the backgate for a sample with a relatively modest mobility (\(\mu = 1700\) cm\(^2\)V\(^{-1}\)s\(^{-1}\)). The \(I-V\) is superlinear at the \(V_g\) of the Dirac point, consistent with the above prediction of ZK tunneling. The superlinearity is better seen in a double-logarithmic scale plot (Fig. 3c) where the \(I-V\) is reasonably well described by a power law \(I \propto V^\alpha\) with \(\alpha = 1.3\). Both \(\alpha\) and the current values are in a remarkable qualitative agreement with calculations given the simplicity of the model as can be seen by comparing Fig. 2c (\(l=1\) µm) and Fig. 3c (\(l=1.1\) µm) for small \(V_g\). More elaborated models (e.g. with a more realistic description of impurities and including electron-phonon scattering) are required to reach a quantitative agreement between theory and measurements.

We observe that the superlinearity vanishes for devices with high \(\mu\). Fig. 3b shows \(\alpha\) (extracted at the Dirac point) as a function of the mobility \(\mu\) of 22 different devices. Indeed, as the mobility increases, \(\alpha\) tends to 1 (corresponding to linear \(I-V\)). In an additional experiment, we introduced defects in a high-mobility graphene device by bombarding it with 10 keV electrons. From Fig. 3b, before bombardment the mobility \(\mu = 7000\) cm\(^2\)V\(^{-1}\)s\(^{-1}\) and the \(I-V\) is linear with \(\alpha = 1.0\). After bombardment \(\mu\) drops to 260 cm\(^2\)V\(^{-1}\)s\(^{-1}\) and the \(I-V\) becomes superlinear (\(\alpha = 1.2\)). These observations are consistent with the above discussion that in high-mobility samples the ZK superlinearity is masked by the non-tunneling current. Namely, the reduction of disorder increases the contribution of the non-tunneling current with respect to the ZK one and, also, favors the non-tunneling current saturation (due to scattering with optical phonons).\(^{18,20}\)

We now discuss other mechanisms that could lead to superlinear \(I-V\)s. It could be related to the physics occurring at tunnel barriers (such as the Luttinger liquid-like behavior in nanotubes or the breakdown of insulating barriers). However, measurements are done on high-quality devices in a four-point configuration, which makes the presence of tunnel barriers unlikely. Superlinear \(I-V\)s could also be attributed to quantum effects, such as weak localization or electron-electron interaction, but these effects should be negligible since the applied current is large, heating the graphene layer to several hundreds of Celsius.\(^{25}\) Overall, Zener-Klein tunneling remains the most plausible mechanism to explain our measurements.

We finally stress that previous observations of Klein tunneling\(^{10,12,13}\) in graphene were done using very different device setups. In\(^{10,12,13}\) the carriers tunnel from conduction to valence bands in a \(p-n\) junction. In these nanostructured devices, the ZK tunneling is observed thanks to a configuration which allows to eliminate the non-tunneling current and thanks to the intense electric field at the \(p-n\) junction (\(\sim 10^3\) eV/Å, see suppl. info of 13 and 5). In our devices, which are not \(p-n\) junc-
tions, the non-tunneling (intraband) current is present (this current can mask the ZK tunneling one) and the electric field (~10^{-5} \text{ eV/Å}) is substantially weaker. Despite these unfavorable conditions, it is possible to probe the Zener-Klein effect.  

Concluding, measurements and calculations show, consistently, that the $I-V$s of graphene devices become superlinear in the presence of disorder (in low-mobility samples). The superlinearity is attributed to Zener-Klein tunneling (tunneling between different energy bands, from $\pi$ to $\pi^*$). In high-mobility (high-quality) graphene samples, the superlinearity is masked by the contribution of the non-tunneling current (due to carriers always remaining the same band). In low-mobility samples, the Zener-Klein tunneling current is visible because the higher density of defects decreases (filters) the non-tunneling current.

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15. We consider a first-neighbors tight-binding electronic Hamiltonian with overlap parameter $t = 3.0 \text{ eV}$ between $\pi$ orbitals ($v_F = 10^8 \text{ cm/s}$) and lattice spacing $a_0 = 2.46 \text{ Å}$. NEGF equations are solved as in Ref. [18] for a strip with length $l = 1 \mu m$ and lateral infinite width. Defect-induced disorder is simulated by changing the on-site potential by $V_0 = 0.1 \text{ eV}$ uniformly on trenches of atoms which are randomly distributed on along the channel. $V_0$ is uniform along the direction perpendicular to the channel (disorder does not break the lateral periodicity) for computational reasons. Long (short) range defects are simulated using trenches long 10$a_0$ ($a_0$). The results are obtained after averaging over various disorder configurations. See [17] for more details. The present approach does not include scattering with optical phonons, which is relevant for $eV > \hbar \omega_l/|\tau_l|$.
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19. Let us write the total current per unit of lateral length as $J = J_{Z} + J_{ZK}$, where $J_{Z}$ and $J_{ZK}$ are the non-tunneling and ZK currents, and let $T = T^{W + R}$ in Eq. [1]. For $eF = 0$, $J_{Z} = 0$ and $J_{ZK} = 2hF/\kappa_0$, where $J_0 = V/(\pi^2 R_d l)$, $R_d = h/(2e^2) = 12.9 \text{ kfl}$, the adimensional quantity $\kappa_0 = V_{tel}/(h\kappa_{el})$, and $F(x) = \sqrt{x} e^x/\xi$. For $l = 1 \mu m$, $\kappa_0 = V/(0.8 \text{ mV})$ and for $V > 0.8 \text{ mV}$ one can show that $J_{ZK} \approx 2h\sqrt{\pi \kappa_0} \sim \pi^{3/2}$. For $eF \neq 0$, let us call $\xi = eV/\epsilon F$. For $\xi < 1$, $J_{Z} = J_{Z}(2 - \xi)\kappa_0$, and for $\xi > 1$, $J_{Z} = 1 - J_{Z}(2 - \xi)\kappa_0$, being $\epsilon = e^2/\pi/(h\kappa_{el})$ the electron concentration. For $\xi < 1$, $J_{Z} = 0$, while for $1 < \xi < 2$, $J_{Z} = J_{Z}(2 - \xi)\kappa_0$, and for $2 < \xi$, $J_{Z} = J_{Z}(2 - \xi)\kappa_0 - \kappa_0$, where the adimensional quantity $\kappa_0 = J_{Z} \pi^2 R_d l/V$ ($\kappa_0 = \kappa_0(\xi - 2)\pi/2$). See [17] for a derivation. Note that the calculated saturation of the non-tunneling current at $eV = eF$ in the ballistic regime ($J_{C} = J_{Z1}$, see Fig. [21]) should not be confused with the saturation due to optical-phonon scattering of [13][23].
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24. Devices were fabricated as in [18] where a graphene sheet is mechanically exfoliated from graphite onto a Si wafer, then structured using dry etching, and finally electrically contacted to metal electrodes in a four-point configuration. Raman spectroscopy and/or measurements of the reflected light intensity with an optical microscope are used to check that the device is a single layer. The current is applied along the channel while $V$ is measured between the voltage electrodes. Measurements are done at 300 K and $10^{-6}$
mbar. \( \alpha \) is obtained from the linear fit of the \( I-V \) in a double logarithmic scale plot for \( V > 0.1 \) V. The mobility is measured as \( \mu = \frac{d\sigma}{dV_g}/C_g \), being \( \sigma(V_g) \) the zero-bias conductivity as a function of \( V_g \). \( \mu \) is measured in the region where \( \sigma(V_g) \) is linear (which is usually attributed to the presence of Coulomb scatterers\(^{25}\)).

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