Full Quantum Time-Dependent Simulation of Electron Devices with Linear 2D Band Structures: Holes or Electrons with Negative Kinetic Energy?

Z. Zhan[1,2], X. Kuang[1], E. Colomés[2],
D. Pandey[2], S. Yuan[1], X. Oriols[2]
[1]*School of Physics and Technology, Wuhan University, Wuhan 430072, China*
[2]*Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193, Bellaterra (Barcelona), Spain*
zhenzhanh@gmail.com, xavier.oriols@uab.cat

During the past years, two-dimensional (2D) materials have been extensively explored to minimize some fundamental challenges encountered in the new-generation of transistors. Some novel physical phenomena, Klein tunneling for example, make the accurate modeling of 2D materials different from that of traditional bulk ones, and need to be properly tackled and flexibly adopted to the device simulator [1,2]. In this conference, a Monte Carlo time-dependent solution of the Dirac equation is presented for full (DC, AC, transient and noise) quantum simulations of electron devices with linear band 2D materials, like graphene in Fig.1 [3,4].

In order to simplify the computational burden of the electron device simulation, carriers with positive kinetic energy are considered as electrons in the conduction band (CB) while carriers in the valence band (VB) are traditionally modelled with the concept of holes (absence of electrons). However, the use of holes in linear 2D materials implies an unphysical treatment of the Klein tunneling process by an *artificial* electron-hole generation, see Fig.2(c). The instantaneous total current $\mathrm{I(t)}$ in the *artificial* Klein tunneling process in Fig.2 (c) is different from that in Fig.2 (b). Consequently, it introduces unphysical results at high-frequency outputs. For instance, the transit time $t_e - t_G$, which determines the cut-off frequency of graphene transistors [5], is much shorter than that of the physical value $t_e - t_0$ in Fig.2(b). This problem simply disappears when treating carriers in the VB as electrons with negative kinetic energy.

In conclusion, the injection of electrons with positive and negative kinetic energies are mandatory to properly simulate the high-frequency electron device characteristics with Klein tunneling in gapless materials like graphene. Numerical results in Figs.3-5 validate the correctness of this *natural* Klein tunneling treatment, which has been implemented in home-made BITLLES simulator (by defining the wave nature of electrons as a bispinor solution of the Dirac equation and its particle nature as a Bohmian trajectory) to study quantum transport for DC, AC and transient in graphene field effect transistors (GFETs).

[1] E. Colomes, Z. Zhan, D. Marian and X. Oriols, Phys. Rev. B, **96**, 075135 (2017).
[2] http://europe.uab.es/bitlles
[3] X. Oriols, Phys. Rev. Lett., **98**, 066803 (2007).
[4] Z. Zhan, X. Kuang, E. Colomes, D. Pandey, S. Yuan and X. Oriols, submitted.
[5] Z. Zhan, E. Colomes and X. Oriols, IEEE Trans. Electron Devices, **64**, 2617 (2017).

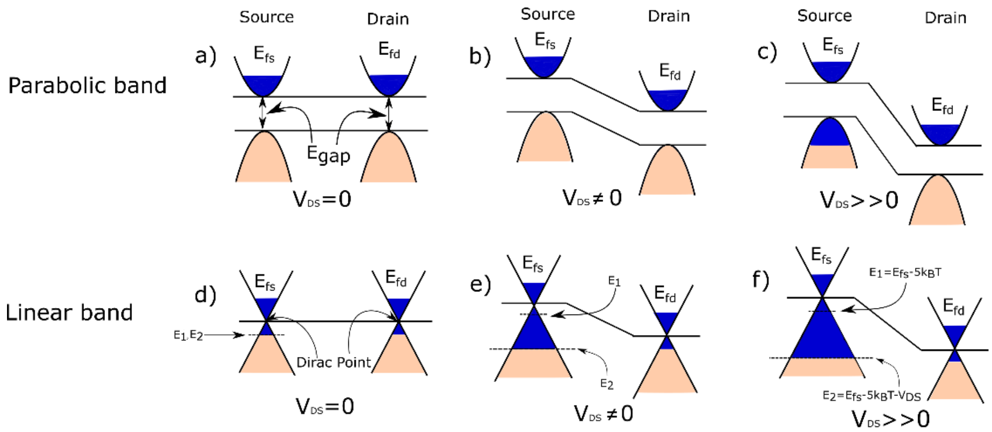
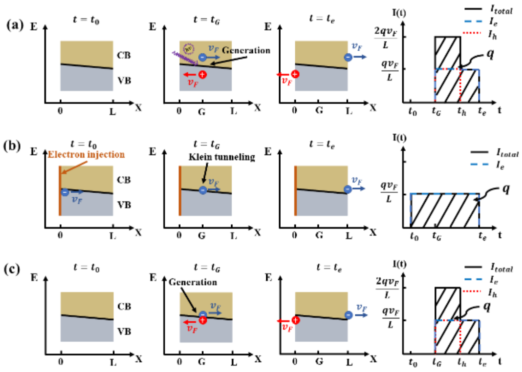


Fig.1: Schematic representation of the energy band structure as a function of the source and drain position for a device with applied bias. The figures (a), (b)and (c) correspond to a device with parabolic CB and VB separated by an energy bandgap E_{gap} with different bias conditions, while the (d), (e) and (f) correspond to a gapless material with linear CB and VB.



Fig,2: Schematic representation of (a) electron-hole generation due to light absorption, (b) Klein tunneling process modeled by one electron injected from the source, traversing from VB to CB, and arriving at the drain contact, (c) Klein tunneling modeled as an electron-hole generation at time t_G at $x = G$. The processes depicted in (a) and (b) provide the correct instantaneous current plotted in the right column. However, when modeling high-frequency properties, unphysical predictions results from the treatment of the Klein tunneling in inset (c).

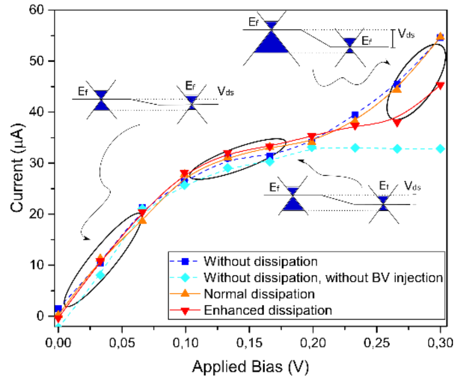


Fig4: Current-voltage characteristic for four dual-gate FETs. The dashed lines depict the ballistic transport where the dark blue (square) one represents graphene injection (electrons injected from both CB and VB) current-voltage characteristic and the light blue (diamond) line represents only electrons injected from the CB. In the orange solid curve, dissipation due to acoustic and optical phonons are taken into account. The red solid line represents enhanced scattering

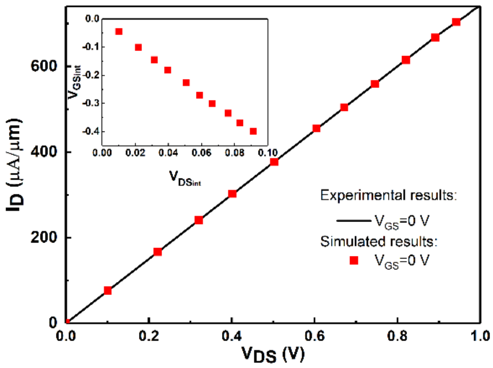


Fig.3: The current-voltage characteristic for a GFET computed (red square) from BITLLES simulator compared with experimental results (black lines). The red square in the inset corresponds to the intrinsic gate-source voltage $V_{GS_{int}}$ and drain-source voltage $V_{DS_{int}}$ used to simulate the drain current I_D in the BITLLES simulator. The simulation and experimental results show quantitative agreement.

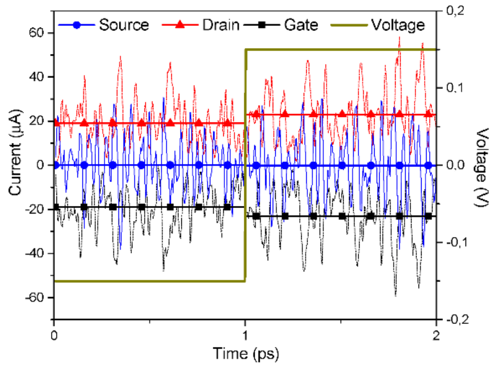


Fig.5: The transient current in a dual-gate FET. Initially both (top and bottom) gate voltages are set to $V_{bg} = V_{tg} = -0.15\ V$, at time $t = 1\ ps$ these values are changed to $V_{bg} = V_{tg} = 0.15\ V$.