Electron injection model for graphene: Is it much different from parabolic-band ones?

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INTRODUCTION

Graphene has many revolutionary properties for fundamental and applied physics. In particular, its linear dispersion implies *unexpected* restrictions for electron dynamics. In time dependent (classical or quantum) particle-based simulators, one needs an algorithm to determine when (and with which properties) electrons are injected from the reservoir into the simulation box [1], [2]. To the best of our knowledge, an electron injection model for graphene is missing in the literature.

PHASE-SPACE DENSITY OF ELECTRONS

A mandatory requirement for an accurate injection model is reproducing the phase-space density [3]. It is well known that the maximum number of electrons, whose positions x, z and wave vectors k_x, k_z fit inside the (2D) phase-space region $\Delta x\Delta K_x\Delta z\Delta K_z$, is $N = g_s g_v \Delta x\Delta K_x\Delta z\Delta K_z/(2\pi)^2$, with g_s spin and g_v valley degeneracies. See Fig. 1.

PHASE-SPACE DENSITY OF INJECTED ELECTRONS

As seen in Fig. 2, when developing an injection model, we are interested in the number of electrons crossing a particular graphene-graphene surface by unit time. In the 2D material, all electrons in the (small) phase-space region $\Delta x\Delta z\Delta K_x\Delta K_z$ move to another spatial region during the time interval $T = \Delta x/v_x$ being v_x the x-component electron velocity. Therefore, the time between injections is:

$$t_o = T/N = (2\pi)^2/(g_s g_v \Delta z\Delta K_x\Delta K_z v_x) \quad (1)$$

where the velocity can be either

$$v_x = v_g k_x/\sqrt{k_x^2 + k_z^2} \quad (linear\ \ dispersion) \quad (2)$$

with $v_g = 3e6\ m/s$ the graphene Fermi velocity, or

$$v_x = \hbar k_x/m \quad (parabolic\ \ dispersion) \quad (3)$$

with $m = 0.9m_o$ the (Silicon) parabolic effective mass. The phase space density of injected electrons defined as $N/T = (t_o)^{-1} \propto v_x$ is plotted in Fig. 3 for parabolic bands and Fig. 4 for linear ones. Almost all graphene electrons moves at the maximum velocity v_g, while a much larger velocity dispersion appears in Silicon.

ALGORITHM IMPLEMENTATION

Since v_x depends on both wave vector components, the graphene electron injection model requires a 2D mesh of the wave vector space, with $K_x = M_x\Delta K_x$ and $K_z = M_z\Delta K_z$. While a 1D mesh is required when (3) is involved. In each cell, the electron velocity is roughly constant. At each simulation time step, from (1), $N = int(T/t_o)$ attempts to inject an electron is done. The injection is successful if the Fermi-Dirac function $f(E_f, E)$ is grater than a random number $r \in [0, 1]$, with E_f the Fermi energy and E the electron energy.

For a very simple ballistic model, the (instantaneous) current computed from $I = qv_x/L_x$ provides dramatic differences between parabolic (Fig. 5(a)) and liner (Fig. 5(b)) band structures. The current dispersion (noise) of both types of dispersion are radically different [4].

CONCLUSION

We present a (time dependent) electron injection model for 2D linear dispersion (graphene) materials. The model includes the thermal noise (and discrete nature of charges) of the reservoir and the injected electrons in the borders of the simulation box satisfy the required phase-space density (faster electrons need to be injected more often than slower ones) [4]. For (classical or quantum) particle-based stimulator of graphene, such injection from a 2D wave vector mesh is mandatory for accurate predictions [5].

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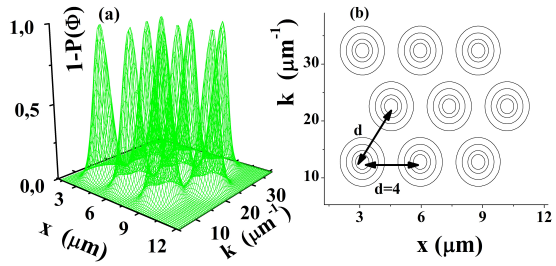

Fig. 1. (a) The presence of N=9 electrons in a region of the 1D phase-space implies that the probability $P(\Phi)$ of N=10 electrons inside this region is almost zero. (b) Contour plot of the right figure where each electron is separated a normalized distance d from the rest [3]. Each electrons requires a phase space region equal to 2π.

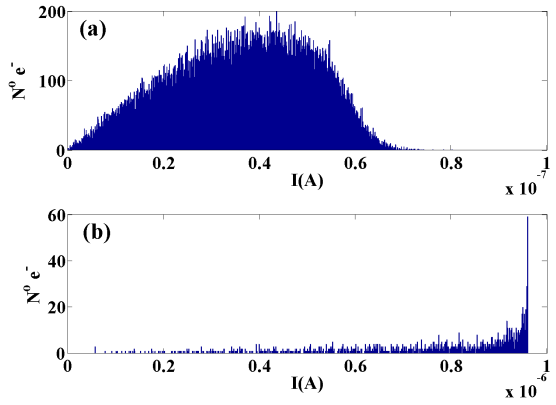

Fig. 5. Number of electrons as a function of instantaneous current I they take during a simulation time of 3.1 ps at 100 K, with Fermi energy $E_f = 0.1\ eV$ for (a) Silicon (b) Graphene. Almost all graphene electrons move at the same velocity and carry the same instantaneous current. We use $g_s = 2$ and $g_v = 1$. This effect has important implications in the intrinsic behavior of AC and noise graphene performances [4], [5].

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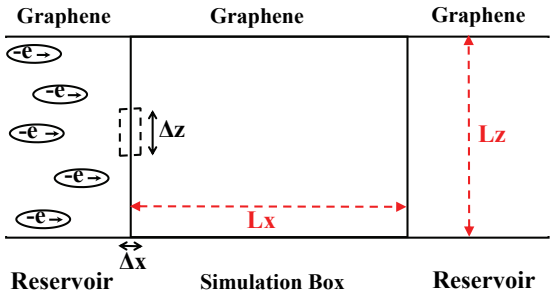

Fig. 2. Schematic representation of the (graphene) reservoir (graphene) simulation box interface where the injection of electrons takes place.

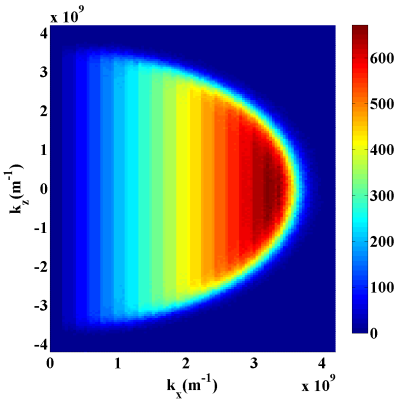

Fig. 3. Number of injected electrons computed from Eq. (1) with $g_s = 2$ and $g_v = 1$ at each point of the 2D wavevector space $\{k_x, k_z\}$ for Silicon during a simulation time of 100 ps at 100 K, with Fermi energy $E_f = 0.1\ eV$. Highest injection rate appears at highest energies. The velocity v_x does only depend on $\{k_x\}$.

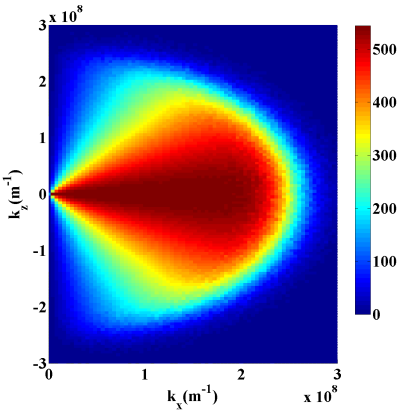

Fig. 4. The same plot as in Fig. 3 for graphene. The highest injection appears in almost all points of the 2D wavevector space $\{k_x, k_z\}$. except those with high k_z [4]. The velocity v_x does explicitly depend on $\{k_x, k_z\}$.