

Analysis of the Electromagnetic/Coherent Transport Problem in Graphene Nanoribbons

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Abstract

The combined quantum and electromagnetic analysis of graphene nanoribbons (GNR), often required for describing applications to practical devices, constitutes a difficult task. Our goal is to develop a multiphysics investigation of the electromagnetic field dynamics together with the quantum coherent transport in nanoscale environment. In this contribution, we show the dynamics of a charge wavepacket from source to drain electrodes in a graphene nanoribbon transistor configuration.

1 Introduction

Graphene is quickly becoming an extremely interesting option for a wide variety of electronic devices and circuits, from low noise amplifiers to non-linear electronics. It offers the possibility of outstanding performances with much lower power draw, using processing technology compatible to that used in advanced silicon device fabrication (CMOS) [1]. Graphene is made of carbon atoms packed in a 2D-honeycomb lattice. Our analysis focuses graphene nanoribbons (GNR), that is, narrow strips of graphene. The analysis of GNR can be carried out by discrete models, such as tight-binding (TB) [2,3], and continuous models, such as effective mass and kp , approximations, which stem from the approximation of TB around particular points of the dispersion curves. The model leads, for the GNR, to a Dirac-like system of equations [2]. Another popular approach for the calculation of quantum transport is given by the use of the Green's function of a GNR region [3-5]. All techniques mentioned above are demonstrated to be quite accurate for the analysis of GNR in a variety of problems such as, for example, the effects on charge transport of applied external electric and magnetic fields [6], bending [7], lattice defects and discontinuities [3], edge terminations [8], and so on [9-10]. Typically, in [2-10], the effects of an external electromagnetic (EM) pulse on a nanodevice is analyzed by considering the internal dynamics of carrier transport as instantaneous with respect to the time constant of the field transient. Often, the ac operation of these quantum devices is computed by making use of an equivalent circuit obtained in the quasi-static limit. A limit of the above methods is that they do not account, dynamically, of the EM field, be it self-consistently generated and/or impressed or external (e.g. impinging plane wave). Recently, we have introduced a novel full-wave time-domain technique aimed at developing a method that accounts for deterministic (EM field) dynamics together with the quantum phenomena [11]. In this technique, the Maxwell equations, defined in a 3D-region and discretized by the transmission line matrix (TLM) method are self-consistently coupled to the Schrödinger equation, describing coherent ballistic transport in a 1D-3D subregion(s) containing the quantum device (carbon nanotubes), and discretized by a proper finite-difference time-domain (FDTD) scheme. As relevant feature, we then introduced [12], immittance boundary operators to account for charge injection and/or absorption from the side metal electrodes contacted to the quantum device. In this contribution, we generalize the concept of the full-wave scheme [11-12] in order to deal with the combined Maxwell-Dirac/graphene equations problem, that is the specific theoretical issue in the presence of graphene as nano-material. The main difference is the nature of the equations describing the quantum device. In the case of a carbon nanotube (CNT), we deal with the Schrödinger equation, that is a complex parabolic diffusion equation; in the case of a graphene sheet, we address the graphene-equations, a particular form of the Dirac equations just for this material, that are hyperbolic equations, isomorphic to the wave equations. A difficulty arises in handling a set of coupled equations, that provide solution in the form of 4-components spinor for the wave-function. In the reported example, we show the space-time evolution of a charge wavepacket propagating along a GNR graphene nanoribbon. We calculate the transmittivity in a source-drain configuration. Finally, we show the effect of the self-generated electromagnetic field, that may affect the group velocity of the charge wavepacket.

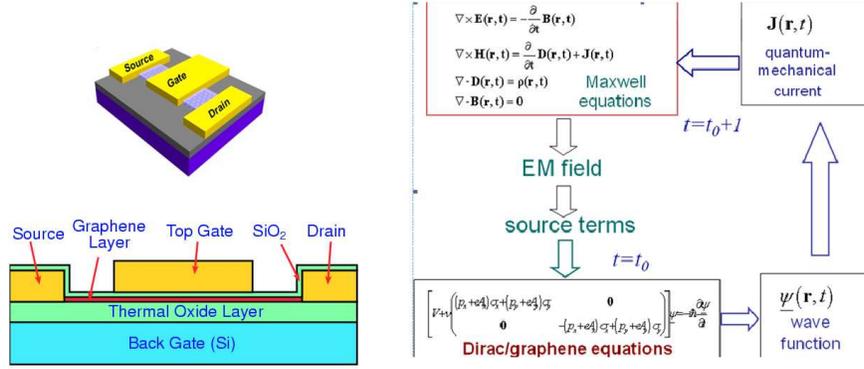


Figure 1: Left-side: scheme of a dual-gate graphene field-effect transistor. Right-side: block scheme of the global full-wave time-domain technique. The electromagnetic field provide sources for the quantum device, that, in turns, provide (quantum-mechanical) current sources for the electromagnetic field.

2 The Multiphysics Time-Domain Scheme

In Fig.1 (left-side), we show a typical configuration of field effect transistor (FET) with a graphene layer as transport channel. In Fig.2 (right-side), we show the concept of the method: inside the three dimensional region, there is a subregion (1D/3D-domain), that is properly the quantum device(s), e.g. a carbon nanotube or nanoribbon. By means of an iteration process, the electromagnetic field provide sources for the quantum device, that, in turns, provide (quantum-mechanical) current sources for the electromagnetic field.

2.1 Modeling of the EM Field

The electromagnetic field dynamics is modeled by using the TLM method. The TLM is a space- and time-discretizing method in which the continuous space is segmented into cells by defining intersecting planes. Ports are defined at the tangential planes between two neighbouring cells and a scattering center is defined at the center of each cell [10-11]. Adjacent nodes are connected by transmission lines and pulses are scattered at the nodes and propagate along these transmission lines to the neighbouring nodes where they are scattered again. The propagation and the scattering of the wave amplitudes are expressed by operator equations; TLM is considered as the implementation of the Huygens principle [11-12].

2.2 Modeling of the Combined EM-Quantum Transport Problem

The concept of the multiphysics computational scheme, depicted in the block scheme of Fig.1 (right side), develops as follows: *i*) the 3D-domain, containing a combination of physical objects (metals, dielectrics, etc...) is discretized by the Transmission Line Matrix method using the Symmetrical Condensed Node (SCN) approach [10]. *ii*) Quantum phenomena are introduced in a subregion of the 3D-domain, e.g. a 1D-2D dimensional CNT region, described by the Schrödinger equation, and/or a 2D-3D graphene-layers region, described by the Dirac equation. As outlined above, a difficulty in dealing with Dirac/graphene equations arise in handling a set of coupled equations, that provide solution in the form of 4-components spinor for the wave-function: $\underline{\psi}(\mathbf{r}, t) = [\psi_1 \ \psi_2 \ \psi_3 \ \psi_4]^T$. *iii*) At an arbitrary time-step t , the electromagnetic (EM) field provides appropriate source terms for the quantum device subregion, by means of the vector and scalar potentials $\mathbf{A}(\mathbf{r}, t)$, $\Phi(\mathbf{r}, t)$, directly calculated from the field components [10]. *iv*) The electromagnetic $\mathbf{A}(\mathbf{r}, t)$, $\Phi(\mathbf{r}, t)$ vector and scalar potentials, respectively, together with the static potential profile, that, in turn, depends on the quantum properties of the device and materials bounding the domain, constitute just additional

source terms for the Schrödinger and/or Dirac (graphene) equations; these equations are then solved by means of the proper finite difference scheme. *v*) The wave solution (spinor) $\underline{\psi}(\mathbf{r}, t)$ generates equivalent quantum-mechanical current $\mathbf{J}(\mathbf{r}, t)$ distributions, that act as a new source for the electromagnetic field at the next $t+1$ time-step [11-12].

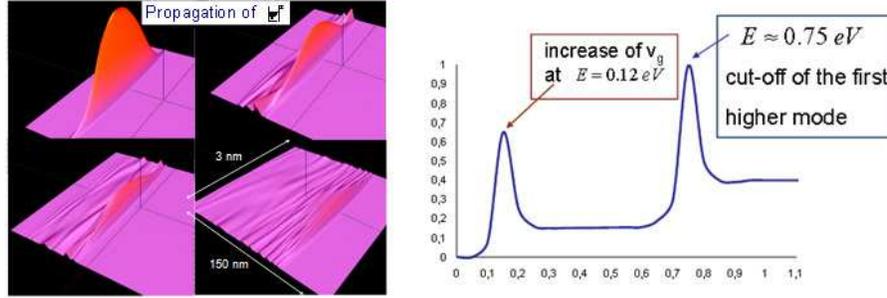


Figure 2: Left-side: graphene nanoribbon with $W = 150 \text{ nm}$ and $L = 3 \text{ nm}$. A space-time Gaussian pulse wavepacket, with energy band up to 1 eV , is injected at the source terminal. Right-side: transmittivity of the analyzed GNR channel of Fig.5, calculated by means of the present technique

3 Example

We analyze a graphene nanoribbon ($W \times L$) with $W = 150 \text{ nm}$ and $L = 3 \text{ nm}$. A space-time Gaussian pulse wavepacket, with broad energy band (up to 1 eV), is injected at the source terminal. Computational parameters, e.g. the elementary Δl space- and Δt time-step, as well as the width σ and amplitude A_0 of the gaussian pulse are directly related to *i*) the energy band, *ii*) the injected charge quantity and *iii*) the geometrical dimensions. The meaning of these parameters are and commented in ref[11-12]. In Fig.2 (left-side), we report the space-time evolution of the injected Gaussian wavepacket, with broad energy band (up to 1 eV), having lateral "metallic boundaries". The kind of boundaries depends on the local orientation of the atoms [10]; the case of "metallic" means that the wavefunction spinor components separately vanish at the lateral sides: $\psi_1 = \psi_3 = 0$ at $x = L$, while $\psi_2 = \psi_4 = 0$ at $x = 0$. In the propagation direction, at the source-drain locations, we model transparent (absorbing) boundary conditions, as in [12]. No static potential barrier is assumed. In Fig.2 (right-side), the transmittivity of the GNR channel is calculated. The first peak corresponds to a change in the group velocity around $E=0.12 \text{ eV}$, the second peak reveals the cut-off of the first higher mode. The physical meaning of these energy values are confirmed by calculating the dispersion curves of the same GNR, by using the tight-binding (TB) technique. In fact, while in two-dimensional graphene the carriers around the Dirac point energy are allowed to travel at $v_F = 10^6 \text{ m/s}$, being the dispersion curve linear, in the case of metallic nanoribbon dispersion curves are become flat towards the Dirac point. This means that carriers propagation is slow ($v < v_F$), up to an energy point (depending on geometrical and constitutive parameters) where dispersion curves are almost linear. We then consider the presence of a static potential barrier ($E=0.45 \text{ eV}$) localized toward the source-drain metal contacts. Now, we consider a static potential barrier, $E=0.45 \text{ eV}$, located at the source-drain terminals. In Fig.3 we calculate the wavepacket space-time propagation without (Fig.3: left-side) and with (Fig.3: right-side) the self-consistent electromagnetic field, for $t=2 \text{ fs}$, $3=4 \text{ fs}$, and $t=6 \text{ fs}$. It is shown how, depending on the initial energy of the wavepacket, the self-induced electromagnetic field affects the propagation characteristics; this is evident by observing the increase of the group velocity, that assumes, in the actual case, values greater the Fermi point velocity ($v > v_F$).

4 Conclusions

We present a full-wave time-domain technique for the combined multiphysics electromagnetic-coherent transport problem in graphene nanoribbons (GNR), where the quantum transport is described by the Dirac equation. The goal of the proposed method is to analyze and predict the relation/coupling between the electromagnetic field dynamics

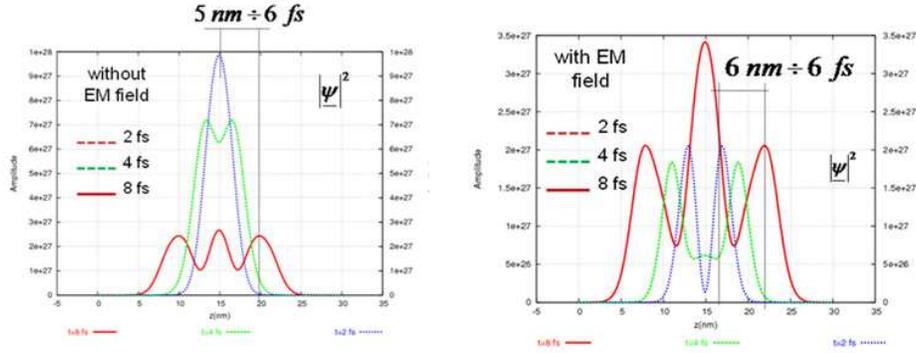


Figure 3: *Left-side: propagation of the charge wavepacket without the self-generated electromagnetic field ($\mathbf{A}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) = 0$), in the presence of a static potential barrier ($E=0.45$ eV) and for $t=2$ fs, $t=4$ fs, and $t=6$ fs. Right-side: propagation of the charge wavepacket with ($\mathbf{A}(\mathbf{r}, t) \neq 0, \Phi(\mathbf{r}, t) \neq 0$) with the self-generated electromagnetic field. The dynamics of the EM field brings the group velocity of the wavepacket beyond the assumed Fermi velocity value.*

and the quantum transport in nanoscale environment. We show the dynamics of a charge wavepacket from source to drain electrodes in a graphene nanoribbon transistor environment. It is shown that the self-induced electromagnetic field affects the charge wavepacket quantum characteristics.

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