Graphene-Based Nano-Antennas for Electromagnetic Nanocommunications in the Terahertz Band

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Abstract—Nanotechnology is enabling the development of devices in a scale ranging from one to a few hundred nanometers. Coordination and information sharing among these nano-devices will lead towards the development of future nanonetworks, boosting the range of applications of nanotechnology in the biomedical, environmental and military fields. Despite the major progress in nano-device design and fabrication, it is still not clear how these atomically precise machines will communicate. Recently, the advancements in graphene-based electronics have opened the door to electromagnetic communications in the nano-scale. In this paper, a new quantum mechanical framework is used to analyze the properties of Carbon Nanotubes (CNTs) as nano-dipole antennas. For this, first the transmission line properties of CNTs are obtained using the tight-binding model as functions of the CNT length, diameter, and edge geometry. Then, relevant antenna parameters such as the fundamental resonant frequency and the input impedance are calculated and compared to those of a nano-patch antenna based on a Graphene Nanoribbon (GNR) with similar dimensions. The results show that for a maximum antenna size in the order of several hundred nanometers (the expected maximum size for a nano-device), both a nano-dipole and a nano-patch antenna will be able to radiate electromagnetic waves in the terahertz band (0.1-10.0 THz).

I. Introduction

Nanotechnology, first envisioned by the Nobel laureate physicist Richard Feynman in his famous speech entitled *"There's Plenty of Room at the Bottom"* in 1959, is giving rise to devices in a scale ranging from one to a few hundred nanometers. The control of matter on an atomic and molecular scale will provide the engineering community with a new set of tools to design and manufacture integrated nano-devices able to perform simple tasks such as local sensing or actuation.

As these devices get more complex, there is the need to control and coordinate their functions, leading to several research challenges in communication at the nano-scale [1]. *Nanocommunications*, i.e., the transmission of information among nano-devices, will expand the capabilities of single devices by means of coordination and information sharing. The resulting *nanonetworks* will boost the range of applications of nanotechnology in the biomedical, environmental and military fields as well as in consumer and industrial goods.
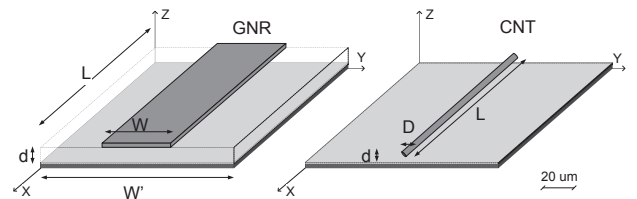
Fig. 1. A nano-patch antenna based on a GNR (left) and a nano-dipole based on a CNT (right).

For the time being, it is still not clear how these atomically precise devices will communicate. Classical communication paradigms need to undergo a profound revision before being used in this new scenario. Focusing on electromagnetic (EM) communications, major progress towards the miniaturization of current EM transceivers has been accomplished up to date. However, there are several limitations in the existing solutions that hamper their direct application in the nano-scale, such as their size, complexity and energy consumption [2], and that raise the question about the feasibility of EM communication among nano-devices. The use of novel nanomaterials as the building block of a new generation of nano-electronic components is envisioned to solve part of the main shortcomings of current technologies. Amongst others, graphene and its derivatives, namely, Carbon Nanotubes (CNT) and Graphene Nanoribbons (GNR), are one of the major candidates to become *the silicon of the 21st century* [3], [4].

From the communication perspective, the electromagnetic properties observed in these materials will determine the specific frequency bands for emission of electromagnetic radiation, the time lag of the emission, or the magnitude of the emitted power for a given input energy. Amongst others, the possibility to manufacture resonant structures in the nano-scale enables the development of novel nano-antennas. A few initial designs based on graphene have been proposed so far. In [5], the mathematical framework for the analysis of carbon nanotubes as potential dipole antennas was developed (Fig. 1 right). In [6], more emphasis was given to the numerical performance analysis of these antennas when compared to classical dipoles. In both papers, the authors do not aim to develop antennas for the nano-scale but advocate for the use of this nano-material in micro- and macro-devices. When it comes to GNRs, the propagation of electromagnetic waves on

a graphene sheet was first analyzed in [7]. In [8], a novel nano-antenna design (Fig. 1 left) based on a suspended GNR and resembling a nano-patch antenna is proposed, modeled, and initially analyzed combining the classical antenna theory with quantum mechanics.

In this paper, a quantum mechanical framework based on the tight-binding model [9] firstly introduced in [8] is extended to carbon nanotubes in order to: i) characterize the transmission line properties of nano-dipole antennas as functions of the CNT dimensions, edge geometry and Fermi energy, ii) obtain relevant antenna parameters such as the the fundamental resonant frequency and the input impedance for nano-dipoles, and iii) compare them to those of a nano-patch antenna with similar dimensions. The results show that for a maximum antenna size in the order of several hundred nanometers (the expected maximum size for a nano-device), both a nano-dipole and a nano-patch antenna will be able to radiate electromagnetic waves in the terahertz band (0.1-10.0 THz).

The remaining of this paper is organized as follows. In Sec. II, the concept behind a CNT-based nano-dipole antenna is reviewed, emphasizing the need for more accurate models for the transmission line properties of CNTs. Then in Sec. III, the tight-binding model is used to obtain the transmission line properties of CNTs as functions of the nanotube dimensions, edge geometry and Fermi energy. Initial numerical results for the expected fundamental resonant frequency and the input impedance of the antenna are obtained in Sec. IV and the paper is concluded in Sec. V.

II. CARBON NANOTUBES AS NANO-DIPOLE ANTENNAS

Carbon nanotubes are one-dimensional molecular structures obtained by rolling up a single graphene sheet into a cylinder, resulting in a Single-Walled Carbon Nanotube (SWCNT), or more than one sheet, resulting in a Multi-Walled Carbon Nanotube (MWCNT). CNTs have several interesting electronic properties, starting from the fact that they can have either a metallic or semiconductor behavior depending on its dimensions and edge geometry [9].

In this work, we think of a lossless metallic SWCNT over a ground plane as a thin-wire center-fed antenna resembling a nano-dipole antenna, as firstly proposed in [5]. Qualitatively, one of the key results in [5] was that a a nanotube antenna would behave in the best case as a short thin-wire antenna with length given by the plasmon wavelength, almost two orders of magnitude smaller than the free-space wavelength. A more accurate conductivity model for CNTs was used in [6], illustrating similar results.

In both cases, the one-dimensional quantum limit was assumed, i.e., only one energy sub-band was considered to be occupied by the electrons in the nanotube. However, only when very thin tubes or very low Fermi energies are considered, this can be assumed. While the final goal will be to have ultra-thin and ultra-low energy nano-devices, we believe that analyzing the effects on the antenna performance introduced when more than one conducting band is occupied deserves some attention. For this, in the next section we use the tight-binding model
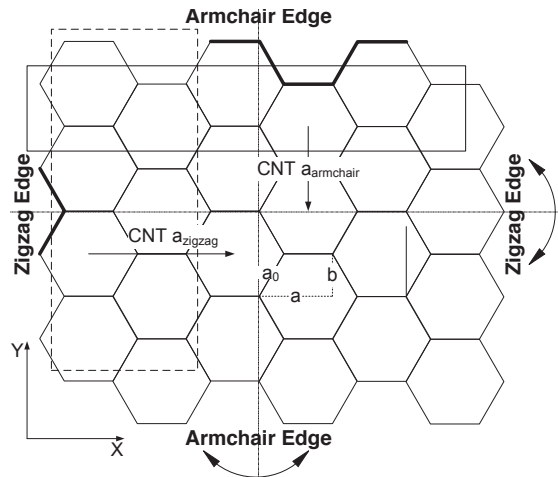

Fig. 2. Lattice structure of a graphene sheet.

to accurately obtain the transmission line properties of CNTs for nano-dipole antennas.

III. TRANSMISSION LINE PROPERTIES OF CNTs

The electronic properties of CNTs strongly depend on their dimensions, Fermi energy and the structure of their edge, which can be mainly either *zigzag* or *armchair* depending on how the graphene sheet is rolled. A generic graphene sheet is illustrated in Fig. 2. In this case, the left and right edges are zigzag edges, whereas the top and bottom edges are armchair edges.

In this section, we first obtain the energy band structure of CNTs with two possible configurations for the edges using the tight-binding model. We then revisit the concepts of quantum resistance, quantum capacitance and kinetic inductance and their dependence on the CNT geometry to obtain the equivalent transmission line properties of carbon nanotubes.

A. Energy Band Structure of Carbon Nanotubes

The electronic band structure of carbon nanotubes, describing the ranges of energy that an electron in the CNT is *forbidden* or *allowed* to have, is obtained by means of the Schrödinger equation [10] which can be rewritten in time-dependent form as follows:

$$\left(-\frac{\hbar^2}{2m_0}\nabla^2 + U(\vec{r}) \right) \psi(\vec{r}) = E\psi(\vec{r}) \quad (1)$$

where $\hbar$ is the reduced Plank's constant, m_0 is the electron mass, $U(\vec{r})$ stands for the potential energy of an electron at position $\vec{r} = (x, y, z)$, $\psi(\vec{r})$ is the wavefunction describing the energy of an electron located at position $\vec{r}$, and E refers to the total energy that an electron has. Solving the Schrödinger equation for a given structure means obtaining the set of eigenfunctions $\psi(\vec{r})$ and eigenenergies E that satisfy (1) for fixed boundary conditions. Alternatively, the Schrödinger equation can be written using matrix notation as follows:

$$[H]\{\psi\} = E\{\psi\} \quad (2)$$

where $[H]$ stands for the Hamiltonian matrix of the system, $\{\psi\}$ is the vectorial form of $\psi(\vec{r})$ and E is the electron total energy.

In order to simplify the complexity of analyzing an atomically large structure, we use the *tight-binding model* [9]. By means of tight-binding modeling, the complexity of solving the Schrödinger equation for the entire structure is reduced to that of solving the matrix equation for a smaller *unit cell* that can generate the entire nanotube. For this, we first identify a structure within the graphene sheet that can be used to replicate the whole nanotube. This unit cell depends on the edge structure of the nanotube edges and how the tube is folded. For an armchair CNT, the set of atoms that compose a possible unit cell is marked in Fig. 2 by using a solid line. This unit cell can easily reproduce an entire armchair CNT using a vector parallel to the y axis. Similarly, a unit cell that can reproduce an entire zigzag nanotube using a vector parallel to the x axis is shown in the same figure using a dotted line. The Hamiltonian matrix for the chosen nanotube is then written as:

$$[h(k)] = \sum_m H_{n,m} e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)} \qquad (3)$$

where $H_{n,m}$ is the individual Hamiltonian matrix accounting for the interactions of a unit cell with itself ($n = m$) and its neighboring cells ($n \neq m$), $\vec{k}$ is the wavevector of the solution to the Schrödinger equation, and $\vec{d}_m - \vec{d}_n$ defines a vector in the direction in which the unit cell is moved to reproduce the structure. In our analysis we consider a single level of electrons at each carbon atom (S-orbitals). For simplicity, we also assume that only the nearest neighbors of an atom, located at a distance equal to the graphene lattice constant a_0 (0.142 nm in graphene), will interact with it. We refer to this interaction as t, which is approximately equal to -2.7 eV in graphene.

As a result, equation (3) is reduced to the addition of three terms. For an armchair nanotube, this is written as:

$$[h^z(k)] = H_{n,n}^z + H_{n-1,n}^z e^{ik_y 2b} + H_{n+1,n}^z e^{-ik_y 2b} \qquad (4)$$

and similarly for the zigzag case this becomes:

$$[h^a(k)] = H_{n,n}^a + H_{n,n-1}^a e^{ik_x 2a} + H_{n,n+1}^a e^{-ik_x 2a} \qquad (5)$$

The electronic band structure of the nanotube can be now obtained by computing the eigenenergies of (4) or (5) for an armchair or a zigzag nanotube, respectively. The *Brillouin zone*, i.e., the area of interest in the wavevector domain, is the region defined as $-\pi \leq k_y 2b \leq \pi$ for an armchair CNT and $-\pi \leq k_x 2a \leq \pi$ for a zigzag CNT. The points of interest in a band structure are those for which the energy bands are close to zero. These illustrate the first energy states that electrons will occupy when the energy of the system is increased.

B. Quantum Resistance

Graphene and its derivatives show almost *ballistic transport* of electrons for relatively large lengths. The resistance of a ballistic conductor in the nanometer scale approaches a limiting value, usually referred as the quantum resistance or contact resistance. For a one-dimensional structure, this is defined as [10]:

$$\mathcal{R}_\mathcal{Q}^1 = h/2e^2 \approx 12.9 \ k\Omega \qquad (6)$$

where h is Plank's constant, e stands for the electron charge and there is a factor of two accounting for the electron spin. When there is more than one conducting band in the nanotube, the total resistance can be approximated by

$$\mathcal{R}_\mathcal{Q}^T \approx h/2e^2 M \qquad (7)$$

where M refers to the number of conducting bands. This number depends on the Fermi energy that is being considered, the temperature of the system, and the width of the nanotube. For a given Fermi energy and temperature, the number of conducting bands increases with the diameter of the nanotube, because the separation among bands is reduced [8].

C. Kinetic Inductance

Inductance has been conventionally defined as the resistance to current change due to Faraday's law, and it represents the energy stored in the magnetic field generated by a current going through the device. However, in a one dimensional structure, the kinetic energy of electrons can be substantially larger than the energy stored in the magnetic field. Due to the degenerative approximation [10], one can assume that all the energy states below the specific Fermi level are occupied and the ones above it are open. This is true for system temperatures close to 0 K and it is a valid approximation in many cases at ambient temperature. For zero current, the number of electrons moving from left to right are the same as those moving in the opposite direction, canceling the impact of each other. To generate a current, some of the left movers must be converted to right movers or vice versa. Because of the Pauli Exclusion Principle [10], the converted electrons have to go to higher energy levels. Hence, as the current increases, the total kinetic energy of electrons increases too.

The kinetic inductance per unit length of a one-dimensional structure is defined as [11]

$$\mathcal{L}_\mathcal{K}^1 = h/4ve^2 \qquad (8)$$

where h is the Plank's constant, v is the electron velocity and e stands for the electron charge. The electron velocity v can be obtained as:

$$v = \frac{1}{\hbar} \frac{dE}{dk} \qquad (9)$$

where $\hbar$ is the reduced Plank's constant, E stands for the electron energy and k is the wavenumber. In a tube with M conducting bands, the kinetic inductances per unit length associated to each one of the bands can be modeled as a set of inductors in parallel. Hence, the total kinetic inductance per unit length becomes:

$$\mathcal{L}_\mathcal{K}^T = \left(\sum_{n=1}^{M} (\mathcal{L}_\mathcal{K}^n)^{-1} \right)^{-1} \qquad (10)$$

Therefore, by increasing the diameter of the nanotube, the number of conducting bands becomes larger, and the total kinetic inductance is decreased. A similar effect is shown when the Fermi energy is increased.

D. Quantum Capacitance

In a one-dimensional structure, in order to add electric charge in the system, one must add electrons to the available quantized states above the Fermi level, as explained by the Pauli Exclusion Principle [10]. This extra energy is modeled using an equivalent quantum capacitance per unit length, whose value for a one-dimensional structure is [11]:

$$\mathcal{C}_{\mathcal{Q}}{}^1 = 4e^2/hv \tag{11}$$

where e is the electron charge, h is the Plank's constant, and v is the electron velocity (9). In a nanotube with M conducting bands, the total quantum capacitance per unit length can be obtained as:

$$\mathcal{C}_{\mathcal{Q}}{}^T = \sum_{n=1}^{M} \mathcal{C}_{\mathcal{Q}}{}^n \tag{12}$$

where the capacitors corresponding to the different bands are considered to be in parallel. Therefore, when increasing the diameter of the nanotube or the system energy, the number of conducting bands increases and this results in a larger quantum capacitance.

E. Line Impedance

To completely characterize the nano-dipole antenna, one should take into account the electrostatic capacitance and the magnetic inductance that will appear between the nanotube and the ground plane. The electrostatic capacitance per unit length between the CNT and the ground plane, $\mathcal{C}_E$, can be calculated as

$$\mathcal{C}_E = \frac{\pi\varepsilon}{cosh^{-1}(d/D)} \tag{13}$$

where ε stands for permittivity of the material between the nanotube and the ground plane, D is the tube diameter and d refers to the separation between the nanotube axis and the ground plane. In what follows, we assume that the ratio between D and d is constant. The total capacitance per unit length can be obtained as,

$$\mathcal{C}^{-1} = \mathcal{C}_E{}^{-1} + \mathcal{C}_{\mathcal{Q}}{}^{T^{-1}} \tag{14}$$

where it has been taken into account that the electrostatic capacitance $\mathcal{C}_E$ (13) and the total quantum capacitance $\mathcal{C}_{\mathcal{Q}}{}^T$ (12) are in series. As discussed before, the quantum capacitance increases with width and energy, thus, the much smaller electrostatic capacitance will dominate the parallel equivalent circuit of both capacitors. Hence, the total capacitance of the system increases with the width and energy of the nanotube.

The magnetic inductance per unit length, $\mathcal{L}_m$, can be obtained from the following relation:

$$\frac{1}{\sqrt{\mathcal{L}_m\mathcal{C}_E}} = \frac{c}{\sqrt{\varepsilon_r}} \tag{15}$$

where c is the speed of light in vacuum and ε_r stands for the relative permittivity of the material between the nanotube and the ground plane. The total inductance per unit length becomes:

$$\mathcal{L} = \mathcal{L}_m + \mathcal{L}_{\mathcal{K}}{}^T \tag{16}$$

where we have taken into account that the magnetic inductance $\mathcal{L}_m$ (15) and the total kinetic inductance $\mathcal{L}_{\mathcal{K}}{}^T$ (10) are in series. As discussed above, the kinetic inductance of a nanostructure decreases with its width and the system energy. Thus, the total inductance of the system decreases with the width and the energy of the nanotube.

Finally, while the different inductances and capacitances are distributed values, the quantum resistance (7) will only appear in the contacts of the nanotube.

F. Wave Propagation Speed

The wave propagation speed in a transmission line can be obtained as:

$$v_p = \frac{1}{\sqrt{\mathcal{L}\mathcal{C}}} \tag{17}$$

where $\mathcal{C}$ refers to the total capacitance per unit length (14) and $\mathcal{L}$ stands for the total inductance per unit length (16). Both the total capacitance and the total inductance depend on the capacitance and the inductance associated to each conducting band ((12) and (10)). The shape and the number of conducting bands depend on the system energy and the geometry of the nano-antenna (1).

IV. Numerical Results

In this section we numerically compute the fundamental resonant frequency and the line impedance of a nano-dipole antenna based on a CNT with multiple conducting bands, as functions of the nanotube dimensions, for the two main types of edge geometries and for different Fermi energies. For each geometry, first the tight-binding model is used to obtain the energy band structure of the CNT. Then, the number of conducting bands is computed and the quantum resistance $\mathcal{R}_{\mathcal{Q}}{}^T$ (7), the kinetic inductance $\mathcal{L}_{\mathcal{K}}{}^T$ (10) and the quantum capacitance $\mathcal{C}_{\mathcal{Q}}{}^T$ (12) are calculated.

In addition, we compare them to those of a nano-patch antenna based on a graphene nanoribbon (GNR), which are obtained using the same framework as proposed in [8]. The main differences between a CNT and GNR, i.e., between folding the graphene sheet or leave it open, comes from the differences in the energy band structure between them, but also from the fact that the electrostatic capacitance between the GNR and the ground plane has a higher impact.

A. Fundamental Resonant Frequencies

The wave propagation velocity inside the CNT depends on the nanotube dimensions, its edge pattern and the Fermi energy of the structure. Following [5], the first resonant frequency of a CNT-based antenna is $f = v_p/2L$, where v_p is the wave propagation velocity in the nanotube (17) and L stands for the nanotube length. In Fig. 3, the first resonant frequency is plot as a function of the CNT diameter, for the two possible edge patterns, and for three different energies. The nanotube length is kept constant and equal to $L=1$ μm. For a very thin nanotube, 4 nm in diameter at most, the resonant frequency will be below 1.17 THz independently of the energy in the nanotube. However, as the diameter is increased, the resonant frequency will non-linearly increase. This is a result of having more energy bands occupied in the nanostructure. A similar
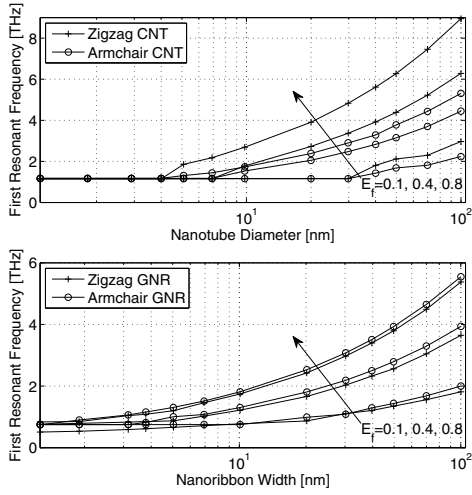
Fig. 3. First resonant frequency of a nano-dipole based on a CNT (top) and a nano-patch based on a GNR (bottom) ($L = 1~\mu m$, E_f in eV).

Fig. 4. Transmission line resistance of a nano-dipole based on a CNT (top) and a nano-patch based on a GNR (bottom) ($L = 1~\mu m$, E_f in eV).

effect happens when the energy of the nanotube is increased. An analogous behavior is seen in a nano-patch antenna when the GNR width is increased. The resonant frequency of a GNR will generally be lower than the CNT. In both cases, for the considered dimensions, a graphene-based nano-antenna will radiate electromagnetic waves in the terahertz band.

B. Input Impedance and Contact Resistance

One of the major shortcomings of the nano-structures envisioned so far is their high contact resistance. Indeed, for a quasi one-dimensional structure such as a nanotube or a very thin nanoribbon, the equivalent resistance measured between their contacts is in the order of 6 kΩ. However, this value can be reduced down to a few hundreds of ohms either by increasing the system energy (the voltage applied to the antenna), or the CNT diameter or GNR width. This agrees with the recent experimental measurements shown in [12].

In Fig. 4, the real part of the input impedance, namely, the resistance of a nanotube antenna $\mathcal{R}_Q{}^T$ (7) is shown as a function of the nanotube diameter, both for a zigzag and an armchair CNT and for different system energies. The tube length is also assumed constant and equal to 1 μm. The input resistance of the nanotube decreases as the number of conducting bands increases. This happens either when the nanotube diameter is increased, which makes the energy bands to be closer, or when the nanotube energy is increased. A similar behavior occurs with the GNR in a nano-patch antenna. In this case, however, the resistance is usually lower than in a nano-dipole because the number of conducting bands increases faster with width.

V. CONCLUSIONS

In this paper we have looked at EM communications among nano-devices and analyzed the use of a lossless metallic single-walled carbon nanotube as a nano-dipole antenna. Using the tight-binding model, we have obtained the energy band structure of different types of CNTs and computed their equivalent transmission line properties. The dependance of the fundament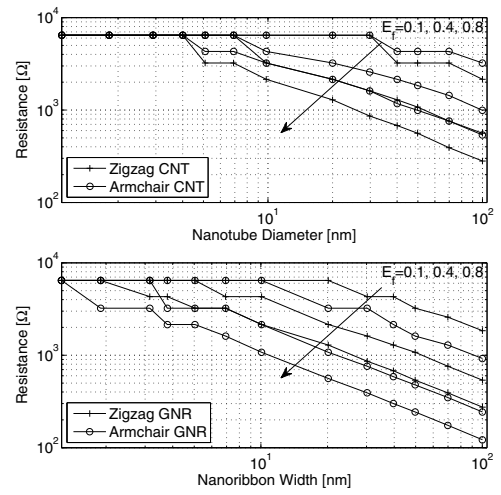al resonant frequency and the antenna input impedance on the nanotube width and the system energy has been analyzed. It has been shown that for a nanotube down to a few nanometers in diameter, the quantum effects govern the wave propagation velocity in the CNT, becoming almost one hundred times lower than the speed of light. When the diameter of the nanotube is increased, the significance of the quantum effects is diminished, and the wave propagation speed tends to the speed of light. In addition, the input impedance of a CNT-based antenna decreases with the nanotube width and system energy. Similar effects were shown for a GNR-based nano-patch antenna. The overall results show that for the size that nano-devices are meant to be, less than one micrometer in any of the dimensions, a graphene-based nano-antenna will be able to radiate EM waves in the terahertz band (0.1-10 THz).

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