Channel Modeling and Capacity Analysis for Electromagnetic Wireless Nanonetworks in the Terahertz Band

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***Abstract*—Nanotechnologies promise new solutions for several applications in the biomedical, industrial and military fields. At the nanoscale, a nanomachine is considered as the most basic functional unit which is able to perform very simple tasks. Communication among nanomachines will allow them to accomplish more complex functions in a distributed manner. In this paper, the state of the art in molecular electronics is reviewed to motivate the study of the Terahertz Band (0.1-10.0 THz) for electromagnetic (EM) communication among nano-devices. A new propagation model for EM communications in the Terahertz Band is developed based on radiative transfer theory and in light of molecular absorption. This model accounts for the total path loss and the molecular absorption noise that a wave in the Terahertz Band suffers when propagating over very short distances. Finally, the channel capacity of the Terahertz Band is investigated by using this model for different power allocation schemes, including a scheme based on the transmission of femtosecond-long pulses. The results show that for very short transmission distances, in the order of several tens of millimeters, the Terahertz channel supports very large bit-rates, up to few terabits per second, which enables a radically different communication paradigm for nanonetworks.**

***Index Terms*—Nanonetworks, channel model, channel capacity, Terahertz Band, molecular electronics, graphene.**

I. Introduction

NANOTECHNOLOGY is enabling the development of devices in a scale ranging from one to a few hundred nanometers. At this scale, a nanomachine is considered as the most basic functional unit which is only able to perform very simple tasks. *Nanocommunication* [1], i.e., the transmission of information among nanomachines, will expand the potential applications of individual devices both in terms of complexity and range of operation. The resulting *nanonetworks* will enable new advanced applications of nanotechnology in the biomedical, environmental and military fields.

Manuscript received April 5, 2010; revised April 7, 2011; accepted July 24, 2011. The associate editor coordinating the review of this paper and approving it for publication was A. Molisch.

This work was supported by the US National Science Foundation (NSF) under Grant No. CNS-1110947, Obra Social "la Caixa" and Fundación Caja Madrid.

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A much shorter version of this work was presented in [23].

Digital Object Identifier 10.1109/TWC.2011.081011.100545

Amongst others, one of the early applications of nanonetworks is in the field of *nanosensing* [2]. Nanosensors are not just tiny sensors, but nanomachines that take advantage of the properties of novel nanomaterials to identify and measure new types of events in the nanoscale. For example, nanosensors can detect chemical compounds in concentrations as low as one part per billion or the presence of virus or harmful bacteria. However, the sensing range of nanosensors is limited to their close nano-environment (usually just a few micrometers) and, in addition, the human interaction and an external device are needed to read their measurements. By means of communication, nanosensors will be able to transmit the sensed information in a multi-hop fashion to a sink or command center. Wireless nanosensor networks will enable novel applications such as advanced health monitoring systems or surveillance systems against Nuclear, Biological and Chemical attacks at the nanoscale, amongst others.

Despite thousands of papers on nano-device technology are being published every year, enabling the communication among nanomachines is still a major challenge. Classical communication paradigms need to undergo a profound revision before being used in nanonetworks. Existing radio frequency (RF) and optical transceivers suffer from several limitations that query the feasibility of electromagnetic (EM) communications among nano-devices, such as their size, complexity and energy consumption [3]. These limitations have motivated the study of new nanomaterials as the basis for a new generation of devices beyond-silicon and next. Amongst others, one of the most promising candidates is *graphene*, a one-atom-thick planar sheet of bonded carbon atoms densely packed in a honeycomb crystal lattice [4], [5]. The unique properties observed in this nanomaterial and its derivatives, Graphene Nanoribbons (GNRs) or Carbon Nanotubes (CNTs), has enabled the development of nano-batteries, nano-processors, nano-memories as well as nano-sensors/actuators [6].

In order to determine the frequency band of operation of future graphene-based EM nano-transceivers, it is necessary to characterize the radiation properties of this nanomaterial. Up to date, several work has been done both from the RF and the optical perspectives. The main difference between the two trends relies on the interpretation of the radiation in terms of high frequency waves or low energy photons. Despite the different origin of the two approaches, they both coincide in the Terahertz Band (0.1-10.0 THz) as the frequency range of operation for the prospect EM nano-transceivers.

In the RF approach, according to the classical antenna

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theory, the reduction of the antenna size down to a few hundreds of nanometers would impose the use of drastically high resonant frequencies. However, at the nanoscale, the propagation of EM waves in graphene is mainly governed by two quantum effects, namely, the quantum capacitance and the kinetic inductance [7]. As a result, the resonant frequency of these nano-antennas can be up to two orders of magnitude below the predicted values. The possibility to define an antenna with atomic precision working at relatively low resonant frequencies opens the door to EM communication for nanonetworks. A few initial designs based on graphene have been proposed so far. In [8], the mathematical framework for the analysis of CNTs as potential dipole antennas was developed. In [9], more emphasis was given to the numerical performance analysis of these antennas when compared to classical dipoles.When it comes to GNRs, the propagation of EM waves on a graphene sheet was first analyzed in [10]. In [11], we compared the performance of novel nano-patch antennas based on GNRs and that of nano-dipole antennas based on CNTs, and we showed that a 1 μm long graphene-based nano-antenna can efficiently radiate EM waves in the Terahertz Band (0.1-10.0 THz). Interestingly enough, this result matches the initial predictions for the frequency of operation of graphene-based RF transistors [12].

From the optical perspective, the emission of photons from nano-structures due to electron-phonon interaction [13], i.e., the interaction between electrons and vibrating ions in the material, motivates the study of nanotubes and nanoribbons as optical emitters (and reciprocally as detectors). From this perspective, the EM radiation is obtained when single electrons collide with the edges of the material in which they are traveling or other particles that can be found in it, releasing photons as a result. In [14], the authors mathematically demonstrate that a quasi-metallic CNT emits Terahertz radiation when a potential difference is applied to its ends. In [15], the absorption of infrared radiation in a nanotube is experimentally demonstrated. Finally, CNTs have been recently proposed as potential optical antennas operating in the Terahertz Band (0.1-10.0 THz) [16], [17]. In light of these results, we advocate for *graphene-based EM nanonetworks in the Terahertz Band*.

In this paper, we focus on EM communications among nano-devices and develop a physical channel model for wireless communication in the Terahertz Band (0.1-10.0 THz). This model allows us to compute the signal path loss, the molecular absorption noise and, ultimately, the channel capacity of EM nanonetworks. We believe our work takes the first step towards formally defining the communication paradigm for nano-devices communicating in the wireless EM spectrum. We summarize the main contributions of our work as follows:

- We develop a channel model for EM nanocommunications in the Terahertz Band by revisiting the concept of molecular absorption and we provide formulations for the total path loss and molecular absorption noise.
- We propose different power allocation patterns for the Terahertz Band and we evaluate the performance of the Terahertz Band in terms of channel capacity.

The rest of this paper is organized as follows. In Sec. II, we develop a new channel model for Terahertz communications by using radiative transfer theory. The capacity of the Terahertz channel and different power allocation patterns are formulated in Sec. III. In Sec. IV, numerical results for the channel path loss, molecular absorption noise and capacity are provided and discussed. Finally, the main conclusions are summarized in Sec. V.

II. Terahertz Propagation Model

Graphene-based EM nano-transceivers will operate in the Terahertz Band, the frequency range in the EM spectrum that spans the frequencies between 100 GHz and 10 THz. While the frequency regions immediately below and above this band (the microwaves and the far infrared, respectively) have been extensively investigated, this is still one of the least-explored zones of the EM spectrum.

The few existing channel models that can be found in the literature [18], [19], [20], [21] are aimed at characterizing the communication between devices that are several meters far, which masks some of the opportunities that the Terahertz Band offers for nanonetworks. The extreme path loss observed for such transmission distances, which is mainly affected by molecular absorption, reduces the total bandwidth to just a few transmission windows, which are several gigahertz wide each. Because of this, current efforts both on device development and channel characterization are focused on the communication in the absorption-defined window arond 300 GHz [22]. However, thinking of the short transmission range of nanomachines, there is a need to understand and model the entire Terahertz Band from 0.1 to 10.0 THz for distances below one meter [23].

In the following, the concept of molecular absorption is reviewed and radiative transfer theory is used to compute the total path loss that a signal suffers when traveling distances in the order of several tens of millimeters or up to a few meters at most. In addition, the effect of molecular absorption on the total system noise is investigated and modeled. The proposed model can take into account the contribution from different types and different concentrations of molecules. As a result, this model can be easily tailored to different scenarios and applications of nanonetworks just by determining the composition of the medium.

A. Molecular Absorption

Several molecules present in a standard medium are excited by EM waves at specific frequencies within the Terahertz Band. An excited molecule internally vibrates, i.e., its atoms show periodic motion while the molecule as a whole has constant translational and rotational motions. As a result of this vibration, part of the energy of the propagating wave is converted into kinetic energy or, from the communication perspective, simply lost. The vibration frequencies at which a given molecule resonates can be obtained by solving the Schrödinger equation for the particular internal structure of the molecule [24]. Alternatively, the necessary parameters to characterize the different resonances for different molecules have extensively collected, contrasted with real measurements, and compiled in either public or private databases [25].

Several methods to predict the molecular absorption for a given medium exist in the microwave region as well as in

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the infrared region. From the radio-frequency perspective, a usual model for the computation of the specific attenuation by gases in the atmosphere between 1.0-1000.0 GHz is the method described in the Recommendation P.676-6 from the International Telecommunications Union [26]. This is obtained in a spectrum line-by-line fashion and only the absorption due to water vapor and oxygen molecules is considered. The main alternatives from the infrared perspective (and the only available option for frequencies above 1 THz) rely on the HITRAN (HIgh resolution TRANsmission molecular absorption database) line catalog [25] or similar databases. While not initially thought for the 0.1-10.0 THz band, this database is found to be a useful asset for the computation of the attenuation due to molecular absorption in our band of interest.

In our analysis, we use radiative transfer theory [27] and the information provided by the HITRAN database to compute the attenuation that a wave traveling distances up to a few meters suffers due to molecular absorption. For this, we first compute the fraction of incident EM radiation at a given frequency that is able to pass through the medium. This parameter is defined as the transmittance of a medium, τ, and is obtained by using the Beer-Lambert Law as:

$$\tau\left(f,d\right)=\frac{P_0}{P_i}=e^{-k(f)d} \tag{1}$$

where f is the frequency of the EM wave, d stands for the total path length, P_i and P_0 are the incident and radiated powers and k is the medium absorption coefficient. This last parameter depends on the composition of the medium, i.e., the particular mixture of molecules found along the channel, and it is defined as:

$$k\left(f\right)=\sum_{i,g}k^{i,g}\left(f\right) \tag{2}$$

where f is the frequency of the EM wave and $k^{i,g}$ stands for the individual absorption coefficient for the isotopologue[1] i of gas g. For example, the air in an office is mainly composed of nitrogen (78.1%), oxygen (20.9%) and water vapor (0.1-10.0%). Each gas has different resonating isotopologues within the Terahertz Band, i.e., molecules that only differ in their isotopic composition.

The absorption coefficient of the isotopologue i of gas g, $k^{i,g}$, in m^{-1}, for a molecular volumetric density, $Q^{i,g}$, in molecules/m^3 at pressure p and temperature T can be written as:

$$k^{i,g}\left(f\right)=\frac{p}{p_0}\frac{T_{STP}}{T}Q^{i,g}\sigma^{i,g}\left(f\right) \tag{3}$$

where p_0 and T_{STP} are the Standard-Pressure-Temperature values and $\sigma^{i,g}$ is the absorption cross section for the isotopologue i of gas g in m^2/molecule. Simply stated, the total absorption depends on the number of molecules of a given gas that are found along the path.

For a given gas mixture, the total number of molecules per volume unit, $Q^{i,g}$, of the isotopologue i of gas g in molecules/m^3, at pressure p and temperature T, is obtained from the Ideal Gas Law as:

$$Q^{i,g}=\frac{n}{V}q^{i,g}N_A=\frac{p}{RT}q^{i,g}N_A \tag{4}$$

[1]A molecule that only differs from another in its isotopic composition.

where n is the total number of moles of the gas mixture that is being considered, V stands for the volume, $q^{i,g}$ is the mixing ratio for the isotopologue i of gas g, N_A stands for the Avogadro constant and R is the gas constant. In the HITRAN database, the contribution of each isotopologue has been scaled according to its natural abundance in the medium. Therefore, the mixing ratio of the specific gas, q^g, should be used for all the isotopologues of g, instead of the individual mixing ratios $q^{i,g}$.

The absorption cross section $\sigma^{i,g}$ in (3) can be further decomposed in terms of the line intensity $S^{i,g}$ for the absorption of the isotopologue i of gas g and the spectral line shape $G^{i,g}$ as:

$$\sigma^{i,g}\left(f\right)=\mathrm{S}^{i,g}G^{i,g}\left(f\right). \tag{5}$$

The line intensity $S^{i,g}$ defines the strength of the absorption by a specific type of molecules and is directly obtained from the HITRAN database. To obtain the line shape, $G^{i,g}$, we first determine the position of the resonant frequency $f_c^{i,g}$ for the isotopologue i of gas g. This increases linearly with the pressure p from its zero-pressure position p_0 as:

$$f_c^{i,g}=f_{c0}^{i,g}+\delta^{i,g}p/p_0 \tag{6}$$

where $f_{c0}^{i,g}$ is the zero-pressure position of the resonance and $\delta^{i,g}$ is the linear pressure shift. All these parameters are directly read from the HITRAN database.

The absorption from a particular molecule is not confined to a single frequency, but spread over a range of frequencies. For a system in which the pressure is above 0.1 atm, the spreading is mainly governed by the collisions between molecules of the same gas [27]. The amount of broadening depends on the molecules involved in the collisions and it is usually referred as the Lorentz half-width $\alpha_L^{i,g}$. We can obtain this parameter as a function of the air and self-broadened half-widths, α_0^{air} and $\alpha_0^{i,g}$ respectively, as:

$$\alpha_L^{i,g}=\left[\left(1-q^{i,g}\right)\alpha_0^{air}+q^{i,g}\alpha_0^{i,g}\right]\left(\frac{p}{p_0}\right)\left(\frac{T_0}{T}\right)^{\gamma} \tag{7}$$

where $q^{i,g}$ is the mixing ratio for the isotopologue i of gas g, p is the system pressure, p_0 refers to the reference pressure, T_0 is the reference temperature, T refers to the system temperature and γ is the temperature broadening coefficient. The values of γ, α_0^{air} and $\alpha_0^{i,g}$ are obtained directly from the HITRAN database. Therefore, the number of molecules does not only increase the amplitude of the peak of the absorption (5), but also makes the shape of the absorption peaks wider, i.e., the useful transmission windows narrower.

For the frequency band that we are considering (relatively low frequencies when compared to the infrared and the light range in which this is usually applied), we choose the Van Vleck-Weisskopf asymmetric line shape [28] to represent the molecular absorption:

$$F^{i,g}\left(f\right)=100c\frac{\alpha_L^{i,g}}{\pi}\frac{f}{f_c^{i,g}}\cdot\left[\frac{1}{\left(f-f_c^{i,g}\right)^2+\left(\alpha_L^{i,g}\right)^2}+\frac{1}{\left(f+f_c^{i,g}\right)^2+\left(\alpha_L^{i,g}\right)^2}\right] \tag{8}$$

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where f stands for the frequency of the EM wave, c is the speed of light in the vacuum, $\alpha_L^{i,g}$ is the Lorentz half-width coefficient for the isotopologue i of gas g and $f_c^{i,g}$ is the resonant frequency for the isotopologue i of gas g.

An additional adjustment to the far ends of the line shape can be done in order to account for the continuum absorption as first proposed in [29]:

$$G^{i,g}(f) = \frac{f}{f_c^{i,g}} \frac{\tanh\left(\frac{hcf}{2k_BT}\right)}{\tanh\left(\frac{hcf_c^{i,g}}{2k_BT}\right)} F^{i,g}(f) \tag{9}$$

where h is the Planck constant, c is the speed of light in the vacuum, k_B stands for the Boltzmann constant and T is the system temperature.

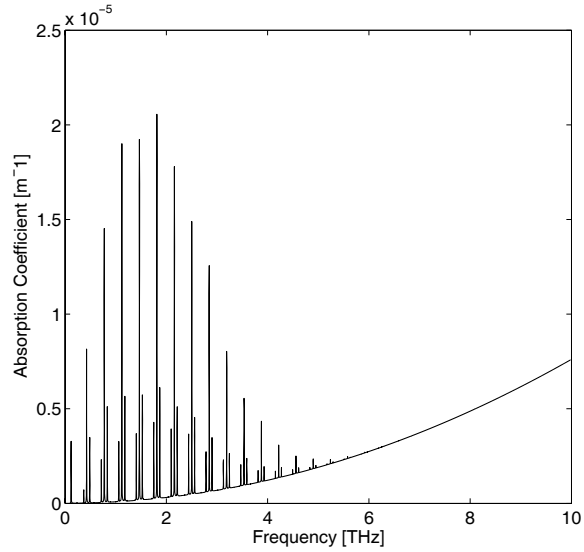
With this, we are able to compute the contributions to the total molecular absorption from each isotopologue i of each gas g present in the medium. As an example, the absorption coefficients for the different isotopologues of oxygen and water vapor molecules are shown as functions of frequency in Fig. 1. Oxygen or O_2 (Fig. 1(a)) has more than two thousand resonances in the Terahertz Band, mainly within 100 GHz and 6 THz. However, the major contribution to the total absorption in a regular medium comes from the molecules of water vapor or H_2O (Fig. 1(b)), with more than four thousand resonant peaks within the entire band, and absorption coefficients six orders of magnitude above those of the oxygen resonances. Rather than the attenuation introduced by fog or raindrops in conventional RF systems in the megahertz and gigahertz spectrums, in the Terahertz Band, the water vapor molecules present in a standard medium already significantly affects the channel performance.

Finally, the total attenuation that an EM wave of frequency f suffers due to molecular absorption when traveling a distance d can be obtained from the transmittance of the medium τ given by (1) as:

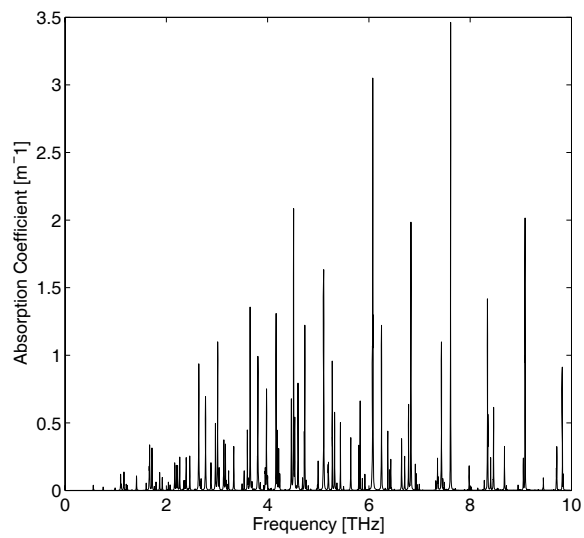
$$A_{abs}(f,d) = \frac{1}{\tau(f,d)} = e^{k(f)d} \tag{10}$$

or in dB

$$A_{abs}(f,d)\,[dB] = k(f)\,d10\log_{10} e. \tag{11}$$



(a) O_2



(b) H_2O

Fig. 1. Molecular absorption coefficient k^g in m^{-1} for oxygen and water vapor as functions of the frequency.

B. Path Loss

The total path loss for a traveling EM wave in the Terahertz Band is obtained as the addition in dB of the spreading loss A_{spread} and the molecular absorption attenuation A_{abs}

$$\mathrm{A}(f,d)\,[dB] = A_{spread}(f,d)\,[dB] + A_{abs}(f,d)\,[dB] \tag{12}$$

where d is the total path length and f stands for the wave frequency. The spreading loss accounts for the attenuation due to the expansion of a wave as it propagates through the medium, i.e., the free-space loss. This is defined in dB as

$$A_{spread}(f,d)\,[dB] = 20\log\left(\frac{4\pi fd}{c}\right) \tag{13}$$

where d is the total path length, f is the frequency of the EM wave and c stands for the speed of light in the vacuum. Within the Terahertz Band, the spreading loss is considerably large, limiting the maximum transmission range of future nano-devices. While this is a major inconvenience for the classical applications for Terahertz communications envisioned so far, we are proposing the use of this band for nanoscale and microscale communications, in which the transmission distance is small, i.e., in the order of several tens of millimeters.

C. Molecular Absorption Noise Temperature

Up to this point, it has been considered that the molecules present in the medium only affect the properties of the channel in terms of attenuation. However, molecular absorption also introduces noise [30]. Indeed, the internal vibration of the molecules turns into the emission of EM radiation at the same frequency that the incident waves that provoked this motion. In our model, we consider this as a noise factor that affects

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TABLE I
MOLECULAR ABSORPTION PARAMETERS AND CONSTANTS

Symbol	Quantity	Units
p	System pressure	[atm]
p_0	Reference pressure	1 atm
T	System temperature	[K]
T_0	Reference temperature	296.0 K
T_{STP}	Temperature at Standard Pressure	273.15 K
V	Volume	[m^3]
n	Total number of moles	[mol]
q^g	Mixing ratio of gas g	[%]
$q^{i,g}$	Mixing ratio of isotopologue i of gas g	[%]
Q^g	Number of molecules per volume unit of gas g	[molecule/m^3]
$Q^{i,g}$	Number of molecules per volume unit of isotopologue i of gas g	[molecule/m^3]
$k^{i,g}$	Absorption coefficient for isotopologue i of gas g	[m^{-1}]
$\sigma^{i,g}$	Absorption cross section of isotopologue i of gas g	[m^2/molecule]
$S^{i,g}$	Absorption peak amplitude of isotopologue i of gas g	[Hz m^2/molecule]
$G^{i,g}$	Spectral lines shape of isotopologue i of gas g	[Hz^{-1}]
$F^{i,g}$	Van Vleck-Weisskopf line shape for isotopologue i of gas g	[Hz^{-1}]
$f_c^{i,g}$	Resonant frequency of isotopologue i of gas g	[Hz]
$f_{c0}^{i,g}$	Resonant frequency of isotopologue i of gas g at reference pressure p_0	[Hz]
$\delta^{i,g}$	Linear pressure shift of isotopologue i of gas g	[Hz]
$\alpha_L^{i,g}$	Lorentz half-width for isotopologue i of gas g	[Hz]
α_0^{air}	Broadening coefficient of air	[Hz]
$\alpha_0^{i,g}$	Broadening coefficient of isotopologue i of gas g	[Hz]
γ	Temperature broadening coefficient	[ ]
h	Planck constant	$6.6262 \cdot 10^{-34}$ J s
k_B	Boltzmann constant	$1.3806 \cdot 10^{-23}$J/K
c	Speed of light in the vacuum	$2.9979 \cdot 10^{8}$ m/s
R	Gas constant	$8.2051 \cdot 10^{-5}$m^{3}atm/K/mol
N_A	Avogadro constant	$6.0221 \cdot 10^{23}$molecule/mol

the propagation of EM waves in the Terahertz Band and we provide a way to compute it.

The parameter that measures this phenomenon is the emissivity of the channel, ε, and it is defined as

$$\varepsilon\left(f,d\right)=1-\tau\left(f,d\right) \tag{14}$$

where f is the frequency of the EM wave, d stands for the total path length and τ is the transmissivity of the medium given by (1).

The equivalent noise temperature due to molecular absorption T_{mol} in Kelvin that an omnidirectional antenna detects from the medium is further obtained as:

$$T_{mol}\left(f,d\right)=T_0\varepsilon\left(f,d\right) \tag{15}$$

where f is the frequency of the EM wave, d stands for the total path length, T_0 is the reference temperature and ε refers to the emissivity of the channel given by (14). This type of noise is only present around the frequencies in which the molecular absorption is considerably high. Water vapor is again the main factor altering the Terahertz channel.

D. Total System Noise Power

Besides the molecular absorption noise, the antenna noise temperature has contributions from several sources, such as the noise created by surrounding nano-devices or the same device per se. To compute the total noise temperature of the system, T_{noise}, the noise introduced by the receiver needs to be taken into account:

$$T_{noise}=T_{sys}+T_{ant}=T_{sys}+T_{mol}+T_{other} \tag{16}$$

where T_{sys} refers to the system electronic noise temperature, T_{ant} is the total antenna noise temperature, T_{mol} is the molecular absorption noise, and T_{other} accounts for any other additional noise source. For the time being, there is no accurate noise model for graphene-based electronic devices, but the initial predictions point to very low noise factors in this nanomaterial [31]. For this, we focus only on the noise introduced by the channel, i.e., the molecular absorption noise.

To compute the equivalent noise power at the receiver, it is necessary to define the transmission bandwidth, which depends on its turn on the transmission distance and the composition of the medium. For a given bandwidth, B, the molecular absorption noise power at the receiver can be calculated as:

$$P_n\left(f,d\right)=\int_B N\left(f,d\right)df=k_B\int_B T_{noise}\left(f,d\right)df \tag{17}$$

where f stands for frequency, d is the transmission distance, N refers to the noise power spectral density (p.s.d.), k_B is the Boltzmann constant and T_{noise} refers to the equivalent noise temperature. Up to this point, we have given formulations to compute the total path loss and the molecular absorption noise power. In the following section, we investigate the capacity of the Terahertz channel by using the developed model.

III. Power Allocation and Channel Capacity

In order to quantize the potential of the Terahertz Band for communication in nanonetworks, we use the channel capacity as a performance metric. In our analysis, we look at the Terahertz Band as a single transmission window almost 10 THz wide. We believe that this is the main new opportunity for communication in nanonetworks.

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Based on the proposed channel model, the Terahertz channel is highly frequency-selective and, in addition, the molecular absorption noise is non-white. Thus, the capacity can be obtained by dividing the total bandwidth into many narrow sub-bands and summing the individual capacities [32]. The i-th sub-band is centered around frequency f_i, $i = 1, 2, ...$ and it has width Δf. If the sub-band width is small enough, the channel appears as frequency-nonselective and the noise p.s.d. can be considered locally flat. The resulting capacity in bits/s is then given by

$$C(d) = \sum_i \Delta f \log_2 \left[1 + \frac{S(f_i) A(f_i, d)^{-1}}{N(f_i, d)} \right] \tag{18}$$

where d is the total path length, S is the transmitted signal p.s.d., A is the channel path loss and N is the noise p.s.d..

The total path loss and the system noise are determined by the frequency of the EM wave, the transmission distance and the molecular composition of the channel, whereas different distributions for the transmitted signal p.s.d. can be adopted. For example, in the simplest case, this is flat over the entire band (0.1 - 10.0 THz),

$$S_{flat}(f) = S_0 \text{ for } f \in B, \text{ 0 elsewhere.} \tag{19}$$

Alternatively, the transmitted signal p.s.d. can be optimally defined to maximize the channel capacity, subject to the constraint that the total transmitted power is finite. For this, the signal p.s.d. S_{opt} should satisfy the water-filling principle:

$$\begin{aligned} &S_{opt}(f) + A(f, d) N(f, d) = K, \text{ and} \\ &S_{opt}(f) = 0 \text{ if } K < A(f, d) N(f, d) \end{aligned} \tag{20}$$

where K is a constant whose value depends on the total transmitted power, which remains as a design parameter in our analysis.

Despite the simplicity or the optimality of these two power allocation schemes, their feasibility can be compromised by the limited capabilities of a single nano-device. Recent advancements in graphene-based nanoelectronics [14], point to the possibility of transmitting very short pulses, just one hundred femtoseconds long. The power of this type of pulses is mainly contained within the Terahertz frequency band. In light of these results, we can envisage a communication technique for nanonetworks based on the exchange of these ultra-short pulses, similar to Impulse Radio Ultra-Wide-Band (IR-UWB) communication systems [33], but for the nanoscale and microscale and in the Terahertz Band. In IR-UWB, tiny bursts of picosecond-long pulses are used with a time between bursts in the order of hundreds of nanoseconds. Orthogonal time hopping sequences are used to interleave different users in a synchronous manner. For nanonetworks, the complexity of such advanced systems is totally out of scope.

In our analysis, we model these pulses as Gaussian-shaped,

$$p(t) = \frac{a_0}{\sqrt{2\pi}\sigma} e^{-(t-\mu)^2/\left(2\sigma^2\right)} \tag{21}$$

where a_0 is a normalizing constant to adjust the pulse total energy, σ is the standard deviation of the Gaussian pulse in seconds, and μ is the location in time for the center of the pulse in seconds. The time derivatives of a Gaussian pulse can be easily obtained by the combination of nanoscale delay lines, and will be also included in the quantitative evaluation of the channel. The p.s.d. of the time derivate of a femtosecond-long pulse is also Gaussian-shaped, but the frequency position of its main components increases with the derivative order n:

$$S_p^{(n)}(f) = (2\pi f)^{2n} a_0^2 e^{-(2\pi\sigma f)^2}. \tag{22}$$

Finally, we will also compute the channel capacity for the case in which a transmission window at 350 GHz with a 51 GHz bandwidth is used. Within this sub-band, the p.s.d., S_{win} is considered flat. This window corresponds to the largest absorption-defined transmission window available when a transmission distance of 10 m is considered. We select window as an illustrative example of macroscale Terahertz communication systems.

IV. Numerical Results

In order to illustrate and understand the different properties of the Terahertz Band from the communication perspective, the proposed channel model is evaluated for different medium compositions, in terms of total path loss, molecular absorption noise and channel capacity. In our analysis, the contributions to molecular absorption from oxygen, carbon dioxide, methane, nitrogen dioxide, ozone, nitrous oxide, carbon monoxide, and water vapor are considered. Their average concentration in a dry atmosphere is used unless the contrary is stated [27].

A. Path Loss

The total path loss, A, given by (12), depends on the EM wave frequency f, the transmission distance d and the composition of the medium that is being considered. In order to illustrate the interrelations between these variables, in Fig. 2, the total path loss is shown in dB as a function of both the frequency (x-axis) and the distance (y-axis) for different concentrations of water vapor molecules. Due to the spreading loss given by (13), the total path loss increases with both the distance and the frequency, independently of the molecular composition of the channel, similarly to conventional communication models in the megahertz or few gigahertz frequency ranges. However, several peaks of attenuation can be observed due to the molecular absorption loss given by (11). As discussed in Sec. II-A, the total absorption depends on the number of molecules that the propagating EM wave encounters before reaching its destination. In a homogeneous channel, this is directly proportional to the molecular cross-section given in (5) and the total path length d.

The main features of the Terahertz Band from the communication perspective are summarized in the following lines:

- The total path loss of a propagating wave in the Terahertz Band does not only depend on the transmission distance and the system frequency, but also on the composition of the transmission medium at a molecular level. In other words, apart from the spreading loss associated to any propagating wave, the presence or absence of absorbent molecules drastically alters the channel behavior. From this, the optimal transmission frequency and its associated bandwidth for a given transmission distance can be determined.

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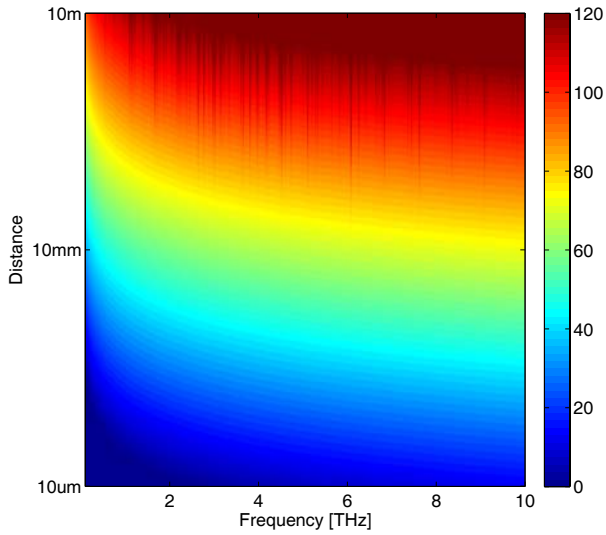
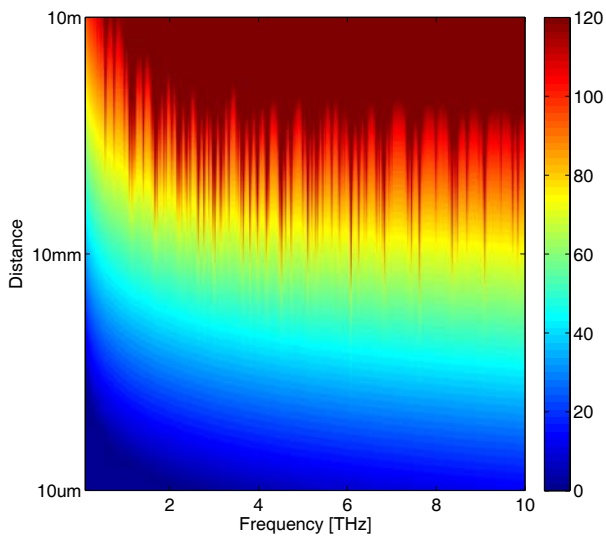
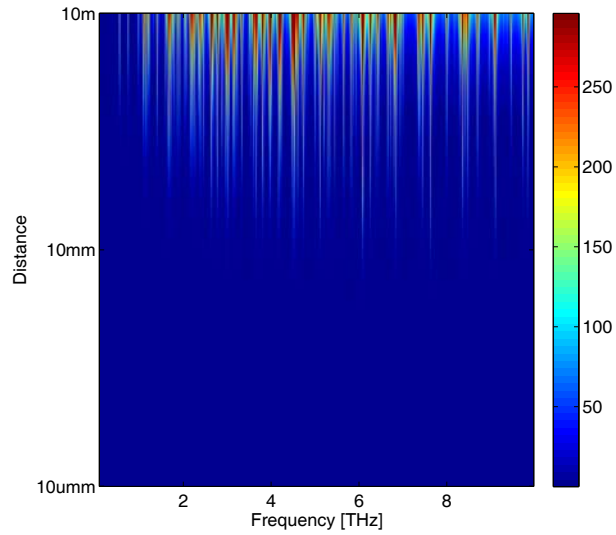


(a) 0.1% H_2O

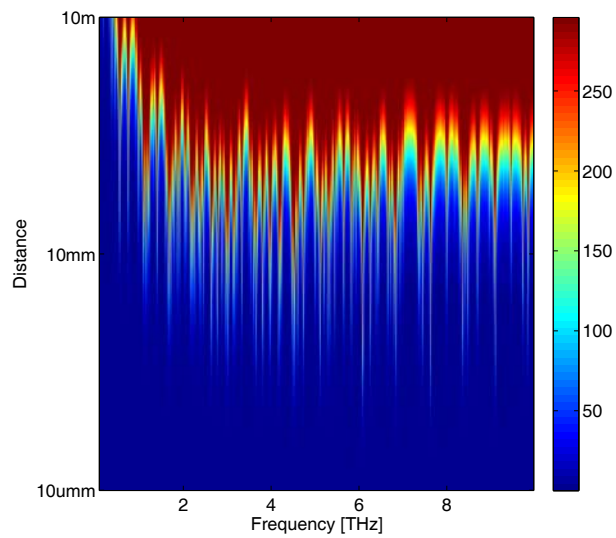


(b) 10% H_2O

Fig. 2. Total path loss in dB as a function of the frequency and the distance for two different concentrations of water vapor molecules (the values for path loss have been truncated at 120 dB to avoid masking relevant transmission windows in the short-range).



(a) 0.1% H_2O



(b) 10% H_2O

Fig. 3. Molecular absorption noise temperature T in Kelvin as a function of the frequency and the distance for two different concentrations of water vapor molecules.

- Within a nanonetwork, it is unlikely to consider single-hop transmission distances above several tens of millimeters. Within this range, the available bandwidth is almost the entire band, from a few hundreds of gigahertz to almost ten Terahertz, even for high concentrations of water vapor molecules, which is the major factor affecting the channel path loss. This opens a wide range of opportunities for communications, from femtosecond-long pulse-based communication systems to multiple access methods based on frequency division techniques. However, note that molecular absorption still determines the frequency response of the channel, and allows, for example, the definition of optimally shaped transmission signals.
- For short-range macroscale communications, i.e., up to a few meters, the channel conditions define a set of transmission windows up to several tens of gigahertz wide each. Current research on Terahertz communication is mainly aimed to exploit the first available window below 350 GHz [19]. The development of graphene-based devices implicitly working in this domain can potentially enable the (simultaneous) use of all them in a cognitive fashion.

These results motivate both, the further analysis of the Terahertz Band and the identification of applications that can benefit from very large bandwidths in the ultra short range.

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B. Noise

The total noise power, P_n given by (17), in a Terahertz communication system depends on the electronic noise temperature at the receiver, T_{sys}, and the molecular absorption noise temperature created by the channel, T_{mol} given by (15). As discussed in Sec. II-C, the electronic noise temperature of the system is expectedly low due to the electron transport properties of graphene. As a result, the main source of noise in the Terahertz Band is the molecular absorption noise introduced by the channel. In the following, taking into account that the computation of the molecular absorption noise power would require the definition of the usable bandwidth B, the molecular absorption noise temperature is calculated instead.

The molecular absorption noise temperature, T_{mol} given by (15), is shown in Fig. 3 as a function of the frequency (x-axis) and the distance (y-axis) for different concentrations of water vapor molecules. In the very short range, the absence of highly absorbent molecules in the medium results in very low noise temperatures. On the contrary, when the number of absorbent molecules that a propagating EM wave encounters along the channel increases, several peaks in the total noise temperature can be observed. The presence of water vapor molecules is again the main factor affecting the properties of the Terahertz channel.

Similarly to the system total path loss, the total system noise defines a set of usable transmission windows which change with the transmission distance between the nano-devices. For the ultra short range, up to several tens of millimeters, the molecular absorption noise power is very low when compared to other noise sources. For the short range, the wise selection of center frequency(s) and bandwidth(s) can diminish the effect of the noise on the system performance.

C. Channel Capacity

The capacity, C given by (18), of the Terahertz channel is determined by the channel path loss, A given by (12), the noise p.s.d., N from (17), and the p.s.d. of the transmitted EM wave. In an intent to keep our numerical results realistic, and in light of the state of the art in molecular-electronics, the total signal energy is kept constant and equal to 500 pJ independently of the specific power spectral distribution. This number is chosen in light of the state of the art in novel energy harvesting systems for nano-devices, such as piezoelectric nano-generators [34], [35], [36]. These mechanisms are able to harvest energy from ambient vibrations, which is then stored in a nano-battery or a nano-ultra-capacitor. These mechanisms have been successfully used to power a laser diode [35] and a PH nanosensor [36]. The maximum amount of energy harvested by these mechanisms depends on several factors, such as the nano-battery size of the frequency of the harvested vibration, but values in the orders of hundreds of nJ have been illustrated. Because of this, we consider that the chosen energy is a reasonable value. However, note that the capacity results presented in this section strongly depend on this value.

1) Channel Capacity for Different Power Allocation Schemes: In Fig. 4, the channel capacity is shown for the four power allocation schemes proposed in Sec. III: the capacity-optimal p.s.d. for the given energy constraint, S_{opt} from (20),

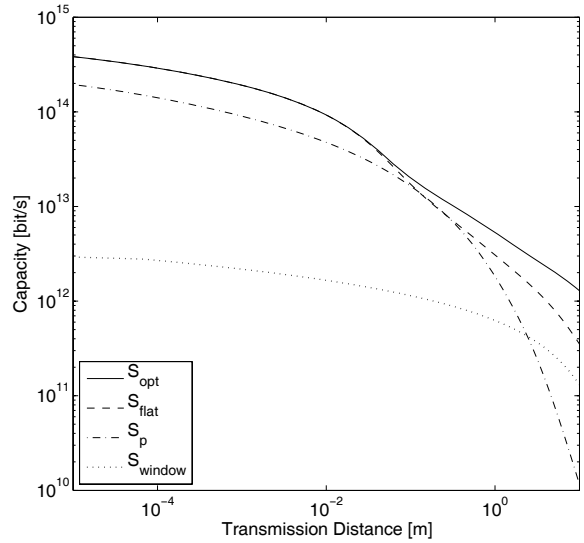

Fig. 4. Capacity as a function of the distance for four different power spectral densities: the capacity-optimal p.s.d., S_{opt}, a flat p.s.d., S_{flat}, the p.s.d. corresponding to the first time derivative of a 100 fs long Gaussian pulse, S_p, and the p.s.d. for the case in which a transmission window at 350 GHz is chosen (1% H_2O).

a uniform distribution of the power within the entire Terahertz Band, S_{flat} from (19), the p.s.d. corresponding to the first time derivative of a 100 fs long Gaussian pulse, $S_p^{(1)}$ from (22), and the p.s.d for the case in which a transmission window at 350 GHz, S_{win}, is used. A standard medium with 1% of water vapor molecules is considered.

For a transmission distance below several tens of millimeters, the molecular absorption is almost negligible. In this case, uniformly distributing the power across the entire band tends to the optimal p.s.d.. On the contrary, by utilizing a single transmission window, even if 51 GHz wide, the capacity in this case would be up to two orders of magnitude below the optimal p.s.d. When the transmission distance is increased, the effect of the molecular absorption is intensified, and uniformly distributing the power along the band is no longer a capacity-efficient option. For a transmission distance on the order of a few meters, utilizing the first transmission window at 350 GHz turns to be the best option. From these results, we also highlight that the exchange of femtosecond-long pulses is a good compromise between achievable information capacity in the Terahertz Band and nano-transceiver architecture complexity.

2) Channel Capacity for Different Molecular Compositions: The channel path loss, A given by (12), and the noise p.s.d., N from (17), are mainly determined by the channel molecular composition. Within the Terahertz Band, the main contribution comes from water vapor molecules. The channel capacity, C given by (18), as a function of the distance for different concentrations of water vapor molecules is shown in Fig. 5 for the optimal power distribution, S_{opt} from (20), and the for the flat p.s.d., S_{flat} from (19), and in Fig. 6, for the p.s.d. corresponding to the first time derivative of a 100 fs long Gaussian pulse, $S_p^{(1)}$ from (22), and for the case in which the first transmission window at 350 GHz is chosen, S_{win}.

The channel capacity of the same EM nanonetwork can

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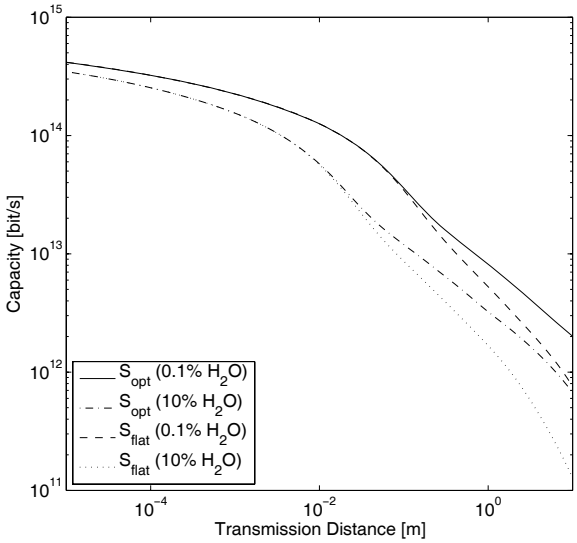

Fig. 5. Capacity as a function of the distance for two different concentrations of water vapor molecules, when the capacity-optimal p.s.d., S_{opt}, and a flat p.s.d. over the entire Terahertz Band, S_{flat}, are used.

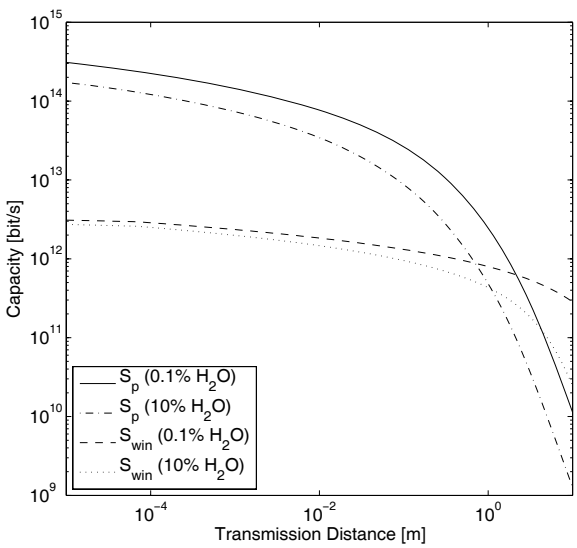

Fig. 6. Capacity as a function of the distance for two different concentrations of water vapor molecules, when the p.s.d. corresponding to the first time derivative of a 100 fs long Gaussian pulse, S_p, and the p.s.d. for the case in which a transmission window at 350 GHz is chosen, S_{win}, are used.

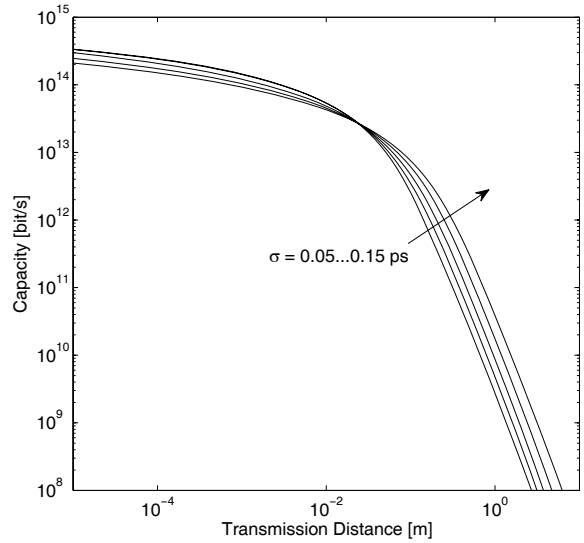

Fig. 7. Capacity as a function of the distance for different pulse-widths, ranging from σ=50 fs to 150 fs, when the p.s.d. corresponding to the first time derivative of a Gaussian pulse, S_p, is used (1% H_2O).

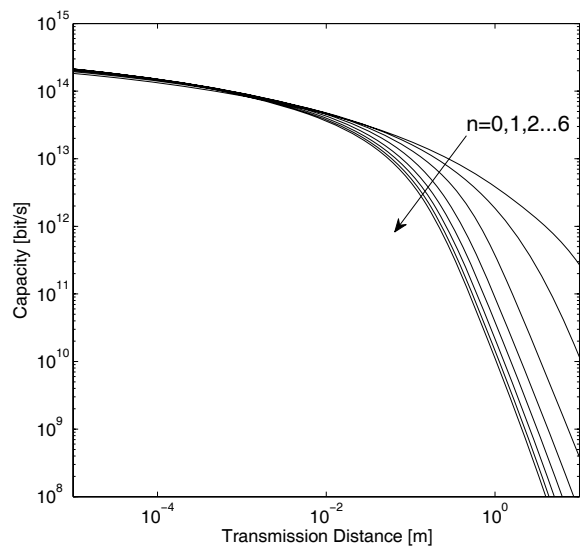

Fig. 8. Capacity as a function of the distance for different derivative orders, ranging from n=0 to 8, when the p.s.d. corresponding to a 100 fs long Gaussian pulse, S_p, is used (1% H_2O).

considerably change depending on the medium conditions. In classical communication channels, the system performance is mainly affected by severe changes in the atmospheric conditions such as fog, rain or snow. In nanonetworks, the limitation on the transmission power and the expected high-sensibility of nanomaterials, make the presence of just a few molecules a major challenge for efficient communication. This effect depends on the total number of molecules found along the channel, and, thus, either when increasing the path length or the concentration of molecules among the path, the performance degradation is similar.

3) Channel Capacity for Different Pulse Shapes: The possibility to generate and transmit femtosecond-long Gaussian pulses by using structures in the nanoscale, invites us to think of a potential communication scheme based on the transmission of ultra-low energy pulses. For a fixed energy, the p.s.d. of a Gaussian-shaped pulse can be modified either by changing its width or by computing its time derivative, which can be obtained by a combination of delay lines.

In Fig. 7, the channel capacity, C given by (18), is illustrated as a function of the distance d, when the p.s.d. corresponding to the first time derivative of a Gaussian pulse, $S_p^{(1)}$ from (22), is used. Different pulse durations, σ, are considered ranging from 50 fs to 150 fs. When the pulse-width is increased,

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the p.s.d. becomes sharper, i.e., the power is concentrated around the center of the Gaussian-shaped pulse. This effect increases the channel capacity for distances above several tens of millimeters, where it has been shown before that it is more efficient to concentrate the power in the lower part of the band. On the contrary, the capacity can be slightly increased in the very short range if shorter pulses are used. Indeed, a shorter pulse has a flatter p.s.d., and this is closer to the shape of the optimal power allocation scheme for the shorter range.

In Fig. 8, the channel capacity, C given by (18), is illustrated as a function of the distance d, when the p.s.d. corresponding to a 100 fs long Gaussian $S_p^{(n)}$ (22) is used, for different time derivative orders n. By computing the time derivative of the pulse, the corresponding p.s.d. is shifted towards the higher part of the band. Taking into account that the total path loss increases with frequency and distance, the channel capacity is reduced with the derivative order, specially for distances above several tens of millimeters. Finally, we would like to highlight that independently of the exact pulse shape, the transmission of very short pulses represents an efficient way to exploit the huge bandwidth provided by the Terahertz Band.

V. Conclusions

Communication among nano-devices will expand the capabilities of limited nanomachines by means of coordination, information sharing and fusion. Nanonetworks will boost the range of applications of nanotechnology in diverse fields ranging from healthcare to homeland security. In this paper, we have advocated for graphene as the enabling technology for future EM nanonetworks in the Terahertz Band (0.1-10.0 THz). We have developed a channel model based on radiative transfer theory to compute the path loss and the noise in the Terahertz Band. Then, we have proposed different power allocation schemes and, finally, we have computed the channel capacity of the Terahertz Band by using the developed channel model.

The results show that Terahertz communication channel has a strong dependence on both the molecular composition of the medium and the transmission distance. The main factor affecting the behavior of the Terahertz Band is the absorption by water vapor molecules, which not only attenuates the transmitted signal, but it also introduces colored noise. In the very short range, i.e., for a transmission distance in the order of several tens of millimeters, the Terahertz Band can be considered as a single transmission window almost 10 THz wide. This is the main difference with existing Terahertz communications systems which are focused on utilizing a single transmission window below 350 GHz.

The very high channel capacity of the Terahertz Band does not only support very high transmission bit-rates, but it also enables new information encoding and modulation techniques as well as novel networking protocols more suited for resource-limited nano-devices. Amongst others, we have suggested the use of femtosecond-long pulses for transmission of information among nanomachines. We acknowledge that there are still several challenges regarding the implementation of a nano-transceiver able to support this communication scheme or its integration in a nanoscale device, but we believe that the expected impact of nanonetworks in our society will definitely motivate and boost its development.

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