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Channel Capacity of Electromagnetic Nanonetworks 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, rising new applications of nanotechnology in the medical, 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. The latest advancements in graphene-based electronics have opened the door to electromagnetic communication among nano-devices in the terahertz band (0.1-10 THz). This frequency band can potentially provide very large bandwidths, ranging from the entire band to several gigahertz-wide windows, depending on the transmission distance and the molecular composition of the channel.**

In this paper, the capacity of the terahertz channel is numerically evaluated by using a new terahertz propagation model, for different channel molecular compositions, and under different power allocation schemes. A novel communication technique based on the transmission of ultra-short pulses, less than one picosecond long, is motivated and quantitatively compared to the capacity-optimal power allocation scheme. The results show that for the very short range, up to a few tens of millimeters, the transmission of short pulses offer a realistic and still efficient way to exploit the terahertz channel.

***Index Terms*—Nanonetworks, Channel Capacity, Terahertz Band, Propagation, Molecular Electronics.**

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 providing the engineering community with a new set of tools to design and manufacture integrated nano-devices able to perform simple tasks such as sensing, computing, data storing, and actuation. As these devices get more complex, there is a need to control and coordinate their functions, leading to several research challenges in communication at the nanoscale [1]. *Nanocommunications*, i.e., the transmission of information among nano-devices, will expand the capabilities of single devices by means of coordination, information sharing and fusion. The resulting *nanonetworks* will boost the range of applications of nanotechnology, bringing new opportunities for bio-medical technology (e.g., cooperative drug delivery systems [5]), environmental research (e.g., distributed air pollution control [9]), or in the military field (e.g., nano-sensor networks for Nuclear, Biological and Chemical (NBC) defenses [6]).

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 nanoscale, such as their size, complexity and energy consumption [13], 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 nanoelectronic 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* [2], [12].

From the communication perspective, the properties observed in these materials will decide on the specific bandwidths for emission of EM radiation, the time lag of the emission, or the magnitude of the emitted power for a given input energy, amongst others. In order to predict the frequency band of operation of future EM nanonetworks (see Fig. 1), it is necessary to characterize the radiation properties of graphene. Up to date, several studies have been conducted both from the radio-frequency [10], [3], [21] and the optical [16], [20], [11] perspectives. The main difference between the two trends relies on the interpretation of the radiation in terms of high frequency resonant waves radiated from nanoscale antennas, or low energy photons radiated from optical nano-emitters. Despite their different origin, both approaches envisage the terahertz band (0.1-10 THz) to become the frequency range of operation for future nano-electromagnetic transceivers.

In this paper we focus on electromagnetic communications in the nanoscale, and numerically evaluate the capacity of the terahertz channel for different channel molecular compositions, and under different power allocation schemes. To the best of our knowledge, this is the first attempt to assess the channel capacity of future electromagnetic nanonetworks in the terahertz band. We summarize the main contributions of our work as follows:

- We first begin with a review of the terahertz channel, emphasizing the challenges posed by molecular absorption, and introduce a novel propagation model.

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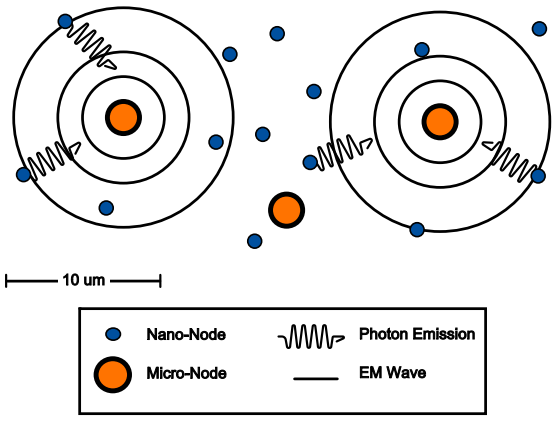

Fig. 1. A nanonetwork based on electromagnetic wireless communications.

- We propose and technologically motivate a communication scheme based on the transmission of ultra-short pulses as a plausible technique to exploit the unique properties of the terahertz channel in the short range.
- We focus on channel capacity and obtain quantitative results for the highly frequency-selective terahertz channel, using different power allocation patterns and for different molecular compositions.

The rest of this paper is organized as follows. In Sec. II, the main properties of the terahertz channel are reviewed and the path-loss and noise models used to compute the channel capacity are formulated. In Sec. III, the capacity of a frequency-selective channel is recalled and a communication scheme based on the transmission of picosecond long Gaussian pulses is motivated and proposed. Sec. IV illustrates the numerical results, providing quantitative measures of the channel capacity in bits/s, for different channel molecular compositions and power allocation schemes. Finally, the main conclusions are summarized in Sec. V.

II. The Terahertz Channel

After nano-device design and manufacturing, the terahertz channel is one of the main aspects that makes the realization of wireless nanonetworks a challenge. This still unlicensed band spans the frequencies between 100 GHz and 10 THz. Despite the major limitations of this band for short and medium range communications [15], the terahertz band offers new opportunities for communication in the nanoscale.

In this section, the main characteristics of the terahertz channel in terms of total path-loss and noise are reviewed. For this, a novel propagation model based on radiative transfer theory [8], and that makes intensive use of the HITRAN (HIgh resolution TRANsmission molecular absorption database) line catalog [17] is used. Despite not originally thought for the terahertz band or the nanoscale, the information contained in the HITRAN database is found to be a useful asset for the computation of the attenuation and noise in our frequency and transmission ranges of interest.

A. Path-loss

The total path-loss, A, for a traveling wave in the terahertz band is defined as the addition of the spreading loss, A_{spread}, and the molecular absorption loss, A_{abs}:

$$A\left(f,d\right)=A_{spread}\left(f,d\right)+A_{abs}\left(f,d\right) \tag{1}$$

where f stands for the wave frequency and d is the total path length. The spreading loss accounts for the attenuation due to the expansion of the wave as it propagates through the medium, and it is defined as

$$A_{spread}\left(f,d\right)=\left(\frac{4\pi fd}{c}\right)^{2} \tag{2}$$

where f is the wave frequency, d is the total path length, and c stands for the speed of light in vacuum.

The absorption loss accounts for the attenuation that a propagating wave will suffer because of molecular absorption, i.e., the process by which part of the wave energy is converted into internal kinetic energy of the excited molecules in the medium. Indeed, several molecules present in a standard medium are excited by electromagnetic radiation at certain frequencies within the terahertz band, converting part of the radiation into internal vibrations. The absorption loss A_{abs} reflects this reduction in the wave energy, and it is defined as:

$$A_{abs}\left(f,d\right)=\frac{1}{\tau\left(f,d\right)} \tag{3}$$

where f stands for the wave frequency, d is the total path length, and τ is the transmittance of the medium. This parameter measures the fraction of incident radiation that is able to pass through the medium and can be calculated using the Beer-Lambert Law as [8]:

$$\tau\left(f,d\right)=e^{-k(f)d} \tag{4}$$

where f is the frequency of the EM wave, d stands for the total path length, 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 path, and it is defined as:

$$k\left(f\right)=\sum_{i,g}k^{i,g}\left(f\right) \tag{5}$$

where $k^{i,g}$ is the individual absorption coefficient for the isotopologue[1] i of gas g. For example, a standard medium is mainly composed of nitrogen (78.1%), oxygen (20.9%) and water vapor (0.1.0-10.0%), and each gas has different isotopologues that resonate at several frequencies within the terahertz band. The major contribution comes from water vapor, which will always be present.

The absorption coefficient of an 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:

$$k^{i,g}\left(f\right)=\frac{p}{p_{o}}\frac{T_{STP}}{T}Q^{i,g}\sigma^{i,g}\left(f\right) \tag{6}$$

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

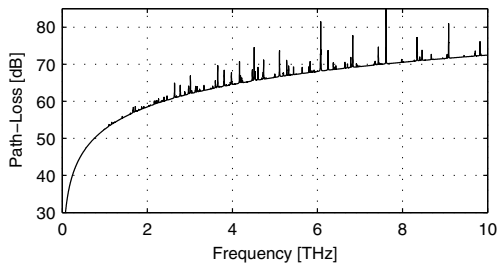

Fig. 2. Total path-loss as a function of frequency for a transmission distance equal to 10 mm, in a standard medium with 1% of water vapor molecules.

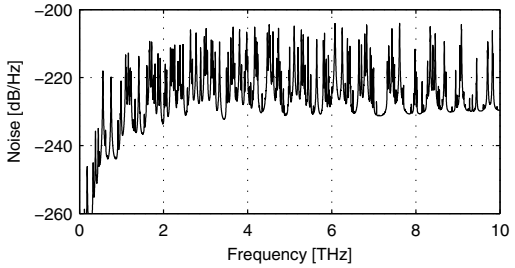

Fig. 3. Molecular noise as a function of frequency, for a transmission distance equal to 10 mm, in a standard medium with 1% of water vapor molecules.

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 will depend 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 of the isotopologue i of gas g per volume unit, $Q^{i,g}$, at pressure p and temperature T, can be obtained from the Ideal Gas Law [18] as:

$$Q^{i,g} = \frac{n}{V} q^{i,g} N_A = \frac{p}{RT} q^{i,g} N_A \tag{7}$$

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.

The absorption cross section $\sigma^{i,g}$ in (6) 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:

$$\sigma^{i,g}(f) = \mathrm{S}^{i,g} G^{i,g}(f) \tag{8}$$

The line intensity $S^{i,g}$ is a parameter directly obtained from the HITRAN database [17]. To obtain the line shape, $G^{i,g}$, we first need to determine the position of the resonant frequency $f_c^{i,g}$ for an isotopologue i of gas g. This increases linearly with the pressure from its zero-pressure position as:

$$f_c^{i,g} = f_{c0}^{i,g} + \delta^{i,g} p / p_0 \tag{9}$$

where $f_{c0}^{i,g}$ is the zero-pressure position of the resonance, p_0 is the reference pressure and $\delta^{i,g}$ is the linear pressure shift. All these parameters are directly read from the HITRAN database [17].

The absorption from a particular molecule is not confined to a single frequency, but is spread over a range of frequencies. For a system in which the pressure is above 0.1 atm, the spreading will be mainly governed by the collisions between molecules of the same gas. The amount of broadening depends on the molecules involved in the collisions and it is usually referred as the Lorentz half-width $\alpha_L^{i,g}$ [8]. This can be obtained as a function of the air and self-broadened halfwidths, α_0^{air} and $\alpha_0^{i,g}$ respectively, as:

$$\alpha_L^{i,g} = \left[(1 - q^g)\, \alpha_0^{air} + q_g \alpha_0^{i,g} \right] \left(\frac{p}{p_0} \right) \left(\frac{T_0}{T} \right)^{\gamma} \tag{10}$$

in which the temperature broadening coefficient γ as well as α_0^{air} and $\alpha_0^{i,g}$ are obtained directly from the HITRAN database [17].

For the terahertz frequency band, an appropriate line shape to represent the molecular absorption is the Van Vleck-Weisskopf asymmetric line shape [19]:

$$F^{i,g}(f) = \frac{\alpha_L^{i,g}}{\pi} \frac{f}{f_c^{i,g}} \cdot \left[\frac{1}{\left(f - f_c^{i,g}\right)^2 + \left(\alpha_L^{i,g}\right)^2} + \frac{1}{\left(f + f_c^{i,g}\right)^2 + \left(\alpha_L^{i,g}\right)^2} \right] \tag{11}$$

An additional adjustment to the far ends of the line shape can be done in order to account for the continuum absorption [4]:

$$G^{i,g}(f) = \frac{f}{f_c^{i,g}} \frac{\tanh\left(\frac{hcf}{2k_B T}\right)}{\tanh\left(\frac{hcf_c^{i,g}}{2k_B T}\right)} F^{i,g}(f) \tag{12}$$

where h is the Planck Constant, c is the speed of light in 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, and consequently, the total molecular absorption loss (3) can be obtained. Molecular absorption makes the terahertz channel highly frequency-selective. As an example, the total path-loss that a wave will suffer when traveling 10 mm in a standard medium with 1% of water vapor molecules, is shown in Fig. 2.

B. Noise

The ambient noise in the terahertz channel is mainly contributed by the molecular noise. The absorption from molecules present in the medium does not only attenuate the transmitted signal, but it also introduces noise. The parameter that measures this phenomenon is the emissivity of the channel, ε, and it is defined as

$$\varepsilon(f, d) = 1 - \tau(f, d) \tag{13}$$

where f is the signal frequency, d stands for the total path length and τ is the transmissivity of the medium (4).

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

$$T_{mol}(f,d) = T_0 \varepsilon(f,d) \tag{14}$$

where T_0 is the reference temperature. This type of noise will only be present around the frequencies in which the molecular absorption is considerably high. As an example, the molecular noise that a propagating wave will create when traveling 10 mm in a standard medium with 1% of water vapor molecules is shown in Fig. 3.

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

$$P_n(f,d) = k_B B\left(T_{mol}(f,d) + T_{other}(f)\right) \tag{15}$$

where f is the wave frequency, d is the total path length, k_B is the Boltzmann constant, B stands for the system bandwidth, T_{mol} refers to the molecular noise temperature and T_{other} is an additional term accounting for any other noise source present in the medium, e.g., electronic noise of the receiver.

III. Power Allocation and Channel Capacity

In order to quantize the potential of the terahertz band for communication in the nanoscale, a performance metric that naturally comes to mind is the channel capacity. The terahertz channel is highly frequency-selective and, in addition, the molecular 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 [7]. The ith 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 power spectral density (p.s.d.) can be considered locally flat. The resulting capacity in bits/s is then given by

$$C(d) = \sum_i \Delta f \log_2\left[1 + \frac{S(f_i) A^{-1}(f_i,d)}{N(f_i,d)}\right] \tag{16}$$

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 signal frequency, 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,

$$S_{flat}(f) = S_0 \text{ for } f \in B, \text{ 0 elsewhere.} \tag{17}$$

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:

$$\begin{aligned} &S_{opt}(f) + A(f,d) N(f,d) = K, \text{ and} \\ &S_{opt}(f) = 0 \text{ if } K < A(f,d) N(f,d) \end{aligned} \tag{18}$$

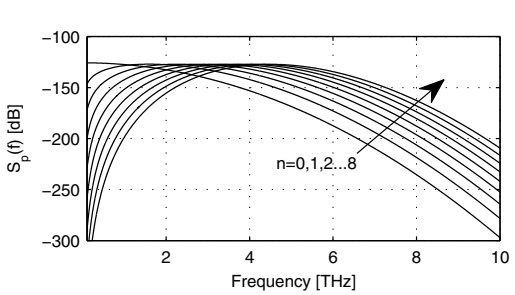

Fig. 4. Power spectral density of a 0.1 ps long Gaussian pulse and its first eight time derivatives (n refers to the derivative order).

where K is a constant whose value depends on the total transmitted power, which will remain 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 nanoscale device. Recent advancements in graphene-based nanoelectronics [16], point out to the possibility of transmitting very short pulses, less than a picosecond 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 nanoscale networks based on the exchange of ultra-short pulses, similar to Ultra-Wide-Band communication systems [14], but for the nanoscale and in the terahertz band. For simplicity, we model these pulses as Gaussian-shaped,

$$p(t) = \frac{a_0}{\sqrt{2\pi}\sigma} e^{-(t-\mu)^2/\left(2\sigma^2\right)} \tag{19}$$

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 p.s.d. of the transmitted pulse, S_p can be obtained as:

$$S_p(f) = a_0^2 e^{-(2\pi\sigma f)^2} \tag{20}$$

The time derivatives of a Gaussian pulse can be easily obtained by the combination of picosecond delay lines, and will be also included in the quantitative evaluation of the channel. The p.s.d. of the time derivate of a picosecond long pulse is also Gaussian-shaped, but the frequency position of its main components increases with the derivative order n (see Fig. 4):

$$S_p^{(n)}(f) = (2\pi f j)^{2n} a_0^2 e^{-(2\pi\sigma f)^2} \tag{21}$$

IV. Performance Evaluation

In this section we quantitatively compare the different power allocation schemes proposed in Sec. III in terms of channel capacity, and for different channel molecular compositions. In an intent to keep these numbers 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 power spectral distribution. For the transmission distance, path lengths ranging from 10 μm to 10 m are considered. In our analysis, the entire terahertz band from 0.1 to 10 THz

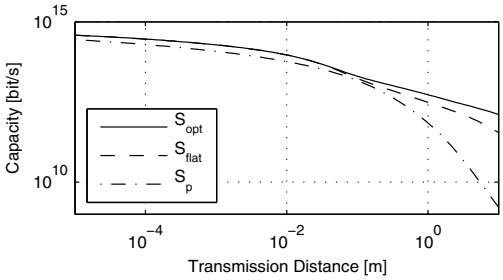

Fig. 5. Capacity as a function of distance for three different power spectral densities: the capacity-optimal p.s.d., S_{opt}, a flat p.s.d., S_{flat}, and the p.s.d. corresponding to the first time derivative of a 0.1 ps long Gaussian pulse, S_p (1 $\%$H$_2$O).

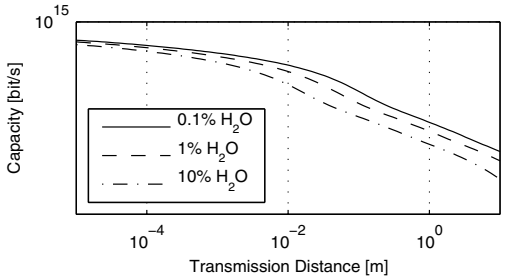

Fig. 6. Capacity as a function of distance for three different water vapor concentrations, when the capacity-optimal p.s.d., S_{opt}, is used.

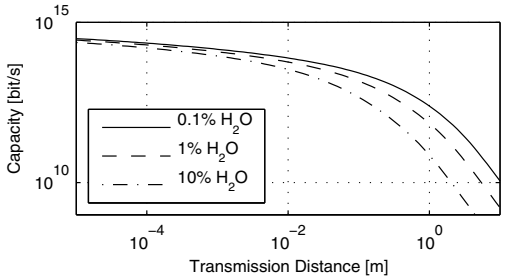

Fig. 7. Capacity as a function of distance for three different water vapor concentrations, when the p.s.d. corresponding to the first time derivative of a 0.1 ps long Gaussian pulse, S_p, is used.

is utilized for the capacity computation. Finally, only the molecular noise (14) is considered in the numerical analysis and, thus, the obtained results serve as an upper-bound for the channel capacity.

A. Channel Capacity for Different Power Allocation Schemes

The capacity of the terahertz channel (16) is determined by the channel path-loss (1), the noise power (15), and the power spectral density of the transmitted signal. In Fig. 5, the channel capacity is shown for the three power allocation schemes proposed in Sec. III: the capacity-optimal p.s.d. for the given energy constraint, S_{opt} (18), a uniform distribution of the power within the band, S_{flat} (17), and the p.s.d. corresponding to the first time derivative of a 0.1 ps long Gaussian pulse, $S_p^{(1)}$ (21). A standard medium with 1% of water vapor molecules is considered.

For a transmission distance below a few tens of millimeters, the molecular absorption is almost negligible, and the differences in the capacity for the three possible power allocation schemes are minimal. Uniformly distributing the power across the entire band tends to the optimal p.s.d. for this transmission range. 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 only the initial absorption-defined window(s) will maximize the channel capacity.

B. Channel Capacity for Different Molecular Compositions

The channel path-loss (1) and the noise power (15) are mainly determined by the channel molecular composition. Within the terahertz band, the main contribution comes from water vapor molecules [15]. The channel capacity as a function of distance (16) for different water vapor concentrations is shown in Figs. 6 and 7, for the optimal power distribution, S_{opt} (18), and the p.s.d. corresponding to the first time derivative of a 0.1 ps long Gaussian pulse, $S_p^{(1)}$ (21), respectively.

The channel capacity of the same nanoscale system can 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 the nanoscale, 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.

C. Channel Capacity for Different Pulse Shapes

The possibility to generate and transmit ultra-short Gaussian pulses using structures in the nanometer scale, invites us to think of a potential communication scheme based on the transmission of ultra-low energy pulses. For a fixed energy, 500 pJ in our analysis, 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. 8, the channel capacity as a function of distance (16), when the p.s.d. corresponding to the first time derivative of a Gaussian pulse, $S_p^{(1)}$ (21), is used, is illustrated for different pulse durations, σ, ranging from 0.05 ps to 0.15 ps. When the pulse-width is increased, 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 a few 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. 9, the channel capacity as a function of distance (16), when the p.s.d. corresponding to a 0.1 ps long Gaussian $S_p^{(n)}$ (21) is used, is shown for different time derivative orders n. As illustrated in Fig. 4, by computing the time derivative of the pulse, the corresponding p.s.d. is shifted

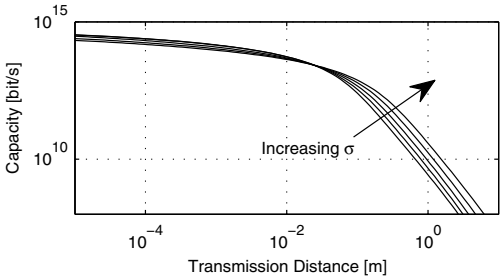

Fig. 8. Capacity as a function of distance for different pulse-widths, ranging from σ=0.05 ps to 0.15 ps, when the p.s.d. corresponding to the first time derivative of a Gaussian pulse, S_p, is used (1 $\%H_2O$).

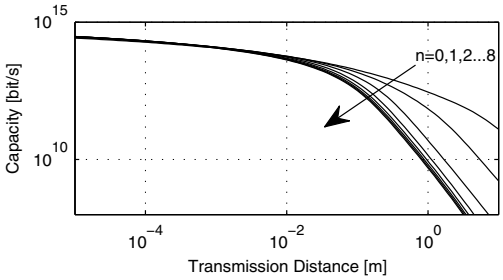

Fig. 9. Capacity as a function of distance for different derivative orders, ranging from n=0 to 8, when the p.s.d. corresponding to a 0.1 ps long Gaussian pulse, S_p, is used (1 $\%H_2O$).

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 a few tens of millimeters.

V. Conclusions

Communication among devices in the order of a few hundred nanometers is envisaged to expand the capabilities of single nano-devices by means of coordination, information sharing and fusion. While the number of applications in which nanotechnology-enabled devices can be used is exponentially increasing, the solutions to the realization of this new communication paradigm are still limited.

In this paper we focus on electromagnetic communications in the terahertz band for future wireless nanonetworks. A new propagation model has been used to characterize the terahertz channel in terms of total path-loss and system noise. The channel capacity of the highly frequency-selective terahertz channel has been obtained as a function of distance and for different power allocation schemes. With an eye towards realistic implementation and in light of the state-of-the-art in molecular electronics, a communication technique based on the exchange of ultra-short range pulses has been proposed. Quantitative results show that this technique can efficiently exploit the ultra-broad band available in the short-range. For distances up to a few tens of millimeters, this scheme can theoretically achieve very high channel capacities, in the order of a few terabits per second.

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