Electronic localization at mesoscopic length scales: different definitions of localization and contact effects in a heuristic DNA model

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Abstract.

In this work we investigate the electronic transport along model DNA molecules using an effective tight-binding approach that includes the backbone on site energies. The localization length and participation number are examined as a function of system size, energy dependence, and the contact coupling between the leads and the DNA molecule. On one hand, the transition from a diffusive regime to a localized regime for short systems is identified, suggesting the necessity of a further length scale revealing the system borders sensibility. On the other hand, we show that the length localization and participation number, do not depend on system size and contact coupling in the thermodynamic limit. Finally we discuss possible length dependent origins for the large discrepancies among experimental results for the electronic transport in DNA sample.

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1. Introduction

The localization of all electronic states in disordered low dimensional systems became a paradigm with the scaling theory of localization over thirty years ago [1]. Nevertheless, this general picture of electronic localization has been challenged by mainly two further developments. On one side, it has been pointed out that correlations in disorder can lead to delocalization. Proposed initially for specific short range correlation [2], it has been shown that a variety of correlations, including long order ones [3], promotes electronic delocalization. On the other hand, the continuous shrinking of solid state devices turned the system size an important length scale. Hence, electronic states normally localized in the thermodynamic limit, encounter a situation in which the localization length
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(LL), is of the order of, or even larger than, the system length [4]. More recently, the possibility of macromolecular systems as a nanoelectronic framework, brought the attention to the electronic properties of DNA strands under a wide range of conditions. The initial results of the search for unraveling the electronic transport properties of DNA [5, 6] caused surprise due to the variety of findings, since DNA appeared to be either an insulator [7–9], a semiconductor [10–13] or a metal [14, 15]. These initially controversial results suggested eventually a complex scenario not yet completely understood. The transport properties of DNA may be affected by a quite long list of effects, either environmental like interaction with substrates, sample dryness, counterions effects; or intrinsic like nucleotide sequencing [16–19]. In order to cope this variety of experimental results, numerous theoretical works of electrical transport through DNA has been extensively studied, ranging from molecular dynamics investigations, through \textit{ab initio} approaches [20, 21], heuristic tight-binding models [22–24], as well as hybrid methods [25], which attempt to bridge the characteristic length scales to the other methods.

These investigation efforts, on its turn, revealed an interesting research stage, where different kinds of disorder, with and without correlations, in systems of variable size in the mesoscopic scale are investigated by means of the same heuristic models once used in numerical studies of electronic localization in the thermodynamic limit. To mention but one of the findings in this scenario, anomalous large LL are encountered for electronic states in double strand (ladder) models in the presence of antisymmetric correlations among on-site energies [26].

This scenario of different kinds of disorder in designed structures at mesoscopic dimensions may challenge the very definition of LL. Indeed, the different definitions of electronic state localization found in the literature, defined in the thermodynamic limit, may show distinct behaviors at mesoscopic system sizes, here an actual relevant length scale. The aim of the present work is to generalize previous findings which suggest an actual wave function extension over an order of magnitude longer than the LL [27]. By comparing the definitions of LL, participation ratio and the sensitivity to boundary conditions [28], an unambiguous estimate of a physical thermodynamic limit length can be defined for a rather general tight binding ladder model [29].

2. Theoretical formulation

In the present work we address one of the various aspects in the long route starting at the investigation of DNA electronic properties, their relations to the transport properties and eventually ending at the proposal of nanoelectronic devices: here we focus on the role of Lead/DNA/Lead coupling strength, as an important parameter for studying the electronic transport through the DNA as function of systems size.

In what follows we describe the general model chosen for this purpose, namely a heuristic model within a tight-binding framework including effective sites for the nitrogenated bases, as well as for sugar and phosphate backbone units, showing relevant
Figure 1. Schematic representation of the DNA ladder model attached to two semi-infinite electrodes at the left (source) and right (drain). The nucleotide base pairs are depicted as blue circles representing the four possible effective nucleotides: A, T, C, and G. Sugar-phosphate (backbone) effective sites are depicted as yellow circles and electronic hoppings are shown as lines. Throughout this work we will consider the limiting case of a completely random sequencing along the central chains, maintaining solely the inter chain base pairing (A-T and C-G).

second nearest neighbor hopping among nitrogenated bases [30, 31]. Such a model captures general physical features of the system under investigation and permits an unambiguous addressing of the localization properties, from a fundamental point of view we are interested in.

A schematic figure of a molecule of DNA coupled to metallic electrodes is shown in Figure 1. In summary, the source and drain electrodes are taken into account using self-energy functions [32]. The coherent transport is studied by computing \( G^r \), the retarded Green’s function, between source and drain, via a recursive lattice Green’s function technique [33]. These are the necessary ingredients which allow us to calculate the density of states (DOS) and the transmission probability (T) used in our analysis of the localization problem.

2.1. The model Hamiltonians

The model tight-binding Hamiltonian depicted in Figure 1 belongs to a standard class of models, widely described in the literature [29], and can be written as:

\[
H_{DNA} = \sum_{l=1}^{L} \left[ \sum_{\alpha=1}^{2} (\varepsilon_{l\alpha} |l, \alpha\rangle \langle l, \alpha| - t_{l,\alpha}^x |l, \alpha\rangle \langle l+1, \alpha|) \\
- t_{l,\alpha}^y |l, \alpha\rangle \langle l+1, \alpha| - t_{l,\alpha}^\sigma |l, \alpha\rangle \langle l, \sigma|) \right] + h.c.
\]  

(1)

The different terms describe the on-site effective orbitals of the nucleotides, the effective sugar and phosphate orbitals and the hopping terms: longitudinal along and transversal to the chains and the crossed (diagonal) hopping between second nearest neighbors nucleotides [30]. Here we follow the hamiltonian description given in a previous work [31].
Hence, $t_{l,\alpha}^x$ is the hopping of base pair $l$ with first nearest neighbors along the strand starting from $5'$ ($j = 1$) and $3'$ ($j = 2$) ends, $t_l^d$ denotes the diagonal hopping and $t_l^y$ the hopping perpendicular from $5'$ down to $3'$ at $l$. The sum over $\sigma$ in equation (1) indicates the connection to the sugar-phosphate backbone. In addition, $\alpha(\sigma) = 1$ (2) for $\sigma = \uparrow$ ($\downarrow$) and $\epsilon_{l\alpha}$ and $\epsilon_l^\sigma$ denote the onsite energies on the 2 DNA strands and the top and bottom backbones.

The onsite energies $\epsilon_{l\alpha}$ are taken to be the effective primary ionization energies of the base nucleotides, i.e. $\epsilon_A = 8.24\text{eV}$, $\epsilon_T = 9.14\text{eV}$, $\epsilon_C = 8.87\text{eV}$ and $\epsilon_G = 7.75\text{eV}$. In this work, we consider the backbone energy to be given as average of the energies of the base nucleotides, i.e. $\epsilon_l^{(\uparrow)} = 8.5\text{eV}$ for all $l$. Both strands of DNA and the backbone are modelled explicitly and the different diagonal overlaps of the larger purines (A,G) and the smaller pyrimidines (C,T) are taken into account by suitable inter-strand couplings [34, 35]. Therefore, couplings are $t_{l,\alpha}^x = 0.35\text{eV}$ between identical bases and $0.17\text{eV}$ between different bases; the diagonal inter-strand couplings are $t_l^d = 0.1\text{eV}$ for purine-to-purine, $0.01\text{eV}$ for purine-pyrimidine and $0.001\text{eV}$ for pyrimidine-to-pyrimidine. The couplings to the backbone sites are $t_l^\sigma = 0.7\text{eV}$, and the hopping across a base pair is $t_l^y = 0.005\text{eV}$. For previous discussions leading to these choices of parameters as well as the influence of the environment on the charge migration properties of the models, we refer the reader to the existing literature [31, 36–38].

This model Hamiltonian is chosen for the reason that, on one hand it grasps the qualitative physics of charge transport in the molecule and, on the other hand it represents a quite general model that can recover simpler ones studied previously throughout the literature.

Nevertheless, we emphasise that the choice of the tight binding parameters is far from uniquely determined, being a rather controversial issue, and several parameter sets have been proposed in the literature [39].

### 2.2. Green function techniques

Having in mind the model Hamiltonian, localization and transport properties are obtained from the transmission probability between the electrodes:

$$T(E) = Tr \left[ \Gamma_S G^r \Gamma_D (G^*)^\dagger \right],$$

(2)

where $G^r$ is the retarded Green function of the system which can be found from [32]

$$G^r = [E - H_{DNA} - \Sigma_S - \Sigma_D]^{-1}.$$  

(3)

The self-energies $\sum_{S(D)} = \tau_{S(D)}^r g_{S(D)} \tau_{S(D)}^d$ and the broadening function $\Gamma_{S(D)} = i \left( \Sigma_{S(D)} - \Sigma_{S(D)}^e \right)$ [32] are calculated as usual from electrode Green’s function $g$ (calculated using a recursive technique [40]) and the coupling $\tau$ between the DNA molecule and electrode. The electrode-molecule coupling $\tau$ is determined by the geometry of the chemical bond [41]. We use couplings ranging [10] from $\tau = 0.35\text{eV}$ to $\tau = 1.5\text{eV}$. 


The diagonal elements of the $\text{Im}[G^r(i,j,E)]$ give us the local density of states (LDOS), another important quantity for investigating the localization properties:

$$\rho(i,j,E) = -\frac{1}{2\pi}\text{Im}[G^r(i,j,E + i\gamma)].$$ \hspace{1cm} (4)

Considering the present open systems and the limit $\gamma \to 0$, one may establish a relation between the LDOS and the electronic probability density: $\rho(i,j,E) = \sum_\alpha \delta(E - \varepsilon_\alpha)|\psi(i,j)|^2$, where $\psi(i,j)$ is defined as the eigenstate with eigenenergy $\varepsilon_\alpha$, of the effective hamiltonian $H = H_{\text{DNA}} + \sum_S + \sum_D$.

3. Localization length and participation number

A further and fundamental step undertaken here is the analysis of the localization of the electronic states. The concept of localization has been originally defined for the thermodynamic limit, but the advent of mesoscopic systems brought new aspects to the understanding of the localization properties. Considering an increasing degree of disorder in a mesoscopic system, the transport can be tuned from ballistic down to the localized regime, with a diffusive transport window between both limits. The LL is a relevant length scale defining these regimes \cite{4}; in particular, one has a localized regime when $L$, the length of the system, is much larger than LL: $L \gg LL$. The diffusive and ballistic regimes are partially characterized by $L \ll LL$. Furthermore, the transition from localized to diffusive transport is rather a wide crossover in the range $L \approx LL$. Hence, the degree of localization for mesoscopic systems has to be carefully investigated. A possible approach is to calculate the LL in the thermodynamic limit and then compare the result with the characteristic length of the mesoscopic system. Such approach, although able to define if the system is far away from the crossover around $L \approx LL$, either in the localized or diffusive regimes, is inconclusive concerning the transition between both regimes. Therefore we analyze here the evolution of different definitions of the degree of localization as a function of the system size in order to identify the transition from localized to diffusive regimes in different DNA-like heuristic models.

The quantities described in the previous section, $T(E)$ and $\rho(i,j,E)$, are relevant ones in defining the localization of a electronic state in the disordered central DNA-like ladder model.

On one hand, LL is computed from the exponential decrease in the transmission probability \cite{42,43}:

$$LL^{-1}(E) = -\lim_{L \to \infty} \frac{1}{2L} < \ln T(E) >,$$

where $< \cdots >$ means an average over several hundred different disordered chain configurations. This is done to avoid spurious resonance effects due to a particular configuration. Here $L$ is the length of the system given in number of bases pairs. Hence, for the sake of completeness in the forthcoming discussion, the total number of effective sites in the system is $4L$. 
Alternatively, another way to define the localization degree of an electronic state is obtained directly from the wave function, namely, the participation ratio, defined initially by [44, 45] for finite systems. Here we define a participation ratio with open boundaries $PR_{OB}$, counting the contributions at each site to the density of states at a given energy:

$$PR_{OB}(E) = \frac{1}{4L} \sum_{i=1}^{4L} \sum_{j=1}^{4} |\rho_{ij}|^2.$$  \hspace{1cm} (6)

For localized states, $PR_{OB} \to 0$ in the limit $L \to \infty$, while truly delocalized states will lead to values up to $PR_{OB} \to 1$. A quantity related to the $PR_{OB}$ is the Participation number (PN), here, $PN=4L \cdot PR_{OB}$. While $PR_{OB}$ is simply a fraction, PN would be a measure of the actual number of sites having appreciable wave-function amplitudes at a given energy.

A final step is the investigation of the effects in changing the coupling of the DNA-like device to the leads. Such investigation is, on one hand, a simple heuristic approach to the effects of the contacts to the leads on the actual transport properties [32]. On the other hand, combining the evolution of different definitions of the degree of localization, as a function of the system size, with the sensitivity to boundary conditions (by changing the contacts), further way to define electronic localization [44], will lead to a comprehensive picture of the electronic state extension properties in mesoscopic length scales.

4. Results and Discussion

A general picture of the question raised in the present work is given by a first comparison between LL and PN, as a function of energy, shown in figure 2 considering two different disordered systems lengths: 30 base pairs (bps) and 300 bps (corresponding to 10.4 nm and 104 nm, respectively). The depicted results here and in the following figures, with the exception of figure 3, are averages over hundreds of disorder configurations. A first main feature is the localization gap, resembling the semiconducting gap introduced by adding backbones to a ladder model, as reported in previous works [38, 46], and absent in simple double chain models [47]. Furthermore, considering the 300 bps long case, all the states are localized, showing a LL an order of magnitude smaller than the system length.

A central issue refers to the differences between the LL, obtained from the transmission probability by means of equation(5), and the PN, obtained as described above, starting from the participation ratio, equation(6). Having in mind that PN is a well defined quantity irrespective to the system size, while LL may be ill defined below the thermodynamic limit, it is worth noting that a gross qualitative agreement between both quantities may be inferred even at the 30 bps case at the upper panel of figure 2. However, from a quantitative point of view, the disagreements are significant. A much
better agreement, both qualitative and quantitative, is obtained for the 300 bps long system.

Two important aspects should be kept in mind for the discussion in the following. (i) The scaling between LL and PN, considering that PN embraces not only the system length, but also the number of chains, not all of them coupled to the contacts and taking part in the transmission. (ii) The quantitative agreement is not uniformly achieved along the entire energy range, particularly at the two anomalously large LL peaks, introduced by the backbones, but also present in other related systems like G4-DNA [48].

A deeper understanding on these aspects and the related definitions of localization is obtained by inspecting of the LDOS for single disorder configurations at chosen values of energy. In figure 3 one can observe the LDOS for single disorder realizations at three energies, $E = -1.05$ eV, $E = -0.74$ eV and $E = -0.58$ eV, which correspond to the highest values of the three peaks in the LL for the valence band in the lower panel of figure 2, i.e., DNA strands 300 bps long. The panels show the LDOS along the system, discriminating the contribution of each of the 4 chains: two chains for the backbones and two constituted by the nucleotides.

All three cases show LDOS with resonances which may appear at any position, sometimes deep inside the system, far from the contacts. From the insets one apprehends that such resonances are indeed very sharp, involving a small number of effective sites. One also observes overall exponentially decaying states from the contacts into the DNA-like double chain with attached backbones, as can be seen from the insets showing the first few base pairs of each case. The tuning of these resonances may enhance dramatically the transmission probability at certain energies for a particular disorder configuration, but, on average, such effects should be washed out. Nonetheless, the
inspection of single disorder configurations reveals that the presence of resonances are quite common, meaning that the incident electronic wave function may couple to states inside the system localized at distances much larger than the scale given by LL. Some configurations, not shown here, may show up to several peaks in the LDOS without a well defined envelope. These findings are qualitatively different from previous ones for bare base pairs ladders (absence of backbones) [27], for which much longer LLs are observed with resonant states spread out over a large number of sites. In spite of these differences, the presence of resonances (in the present case, the resonances are sharpened
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Figure 4. (color online): Localization length (LL)(left panel) and participation number (PN) (right panel) as a function of double-chain length for different double-chain to contact coupling strengths, $\tau$, at $E=-0.74$ eV, corresponding to the highest LL in the valence band in figure 2. The chain lengths are given in units of bps, as well as in nanometers, and the coupling strengths considered are: $\tau = 0.35$ eV (red) $\tau = 1$ eV (blue) and $\tau = 1.5$ eV (green). The shaded areas ($\text{LL} < L$ and $\text{PN} < L$) correspond to the localized regime, while effective delocalization occur at the white areas.

by the presence of the backbones), raises the question of defining a new length scale, given by $L_{wf} > \text{LL}$, which may elucidate the effect of resonance coupling on the effective localization of states.

The closer quantitative agreement between PN and LL for longer systems suggests that the effect of such resonances become progressively less important with increasing system length. Therefore, the transition from short to longer systems, concerning the degree of localization has to be carefully investigated, as illustrated in figure 4, where LL (left panel) and PN (right panel), as a function of the system length at the energy of the highest LL peak at the valence band in figure 2, are shown. The different curves are for different intensities of the coupling to the contacts, introducing the sensitivity to the boundary conditions and, therefore, a size scaling analysis. Several aspects can be appreciated in these results. First of all, differently than for other related heuristic models [27] there is no window of effective delocalization, as can be observe that the numerical results for the degree of localization never reach the white region where the LL would be larger than the system size. On the other hand, the results for LL and PN become length independent at lengths beyond 1000 bps. Two other aspects may call the attention here. First, the LL initially increases with the system length, reaching a maximum and saturating at a lower value at the thermodynamic limit, which for the present case is reached at 300 nm (upper scale of the left panel in figure 4). Second, the PN shows a steady increase with the system length, but never reaching the necessary steepness (dashed line at the right panel) representing effective delocalization. Furthermore, it is also noticeable that the sensitivity to the contact coupling is relevant up to lengths of hundreds of bps, the results becoming insensitive to the coupling intensity for lengths beyond 1000 bps.
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Figure 5. (color online): Localization length (LL) (left panel) and participation number (PN) (right panel) as a function of double-chain length, at $E=-0.74 \text{ eV}$, for different concentrations of G nucleotides: 25% (black), 50% (blue), 75% (red), 95% (green) and 100% (violet), ranging hence from strong disorder (25% and 50%) to almost ordered (95%) and completely ordered (100%). The shaded areas (LL $\leq$ L and PN $\leq$ L) correspond to the localized regime, while effective delocalization occur at the white areas.

From the point of view of actual transport measurements in DNA systems, the coupling to the contacts sensitivity of the LL, a quantity directly related to the transmission probability, is expected to be of relevance within a manifold of other environmental variables. This apparently obvious statement becomes more involved when one also observes the strong dependence of the PN on the contact coupling, since variations in the PN suggest modifications in the LDOS distribution at the given energy, hence the charge distribution in the system.

The results shown in figure 4 suggest that three ways of defining the degree of localization reach insensitivity in respect to the system size at roughly the same system size, defining a the thermodynamic limit in this context of 300 nm, i.e., within a mesoscopic length scale.

A transition from localized to diffusive transport regime would imply in a crossing of LL from the grey to the white area, or a PN showing the same steepness of the dashed border line, in figure 4 for a certain length range. Evidences of such behavior appear in other related models [27] characterized by quite longer LLs, but are clearly absent here. Nevertheless, the disorder considered here is the completely random choice of nucleotides, solely constrained by base pairing, hence there is on average a 25% concentration of each of the bases, A,T,C and G. By increasing the concentration of G, for instance, the degree of disorder may be reduced, reaching eventually an ordered system at the limit of 100% concentration of G. This dependence to the degree of disorder is shown in figure 5 where LL and PN are depicted as a function of size, for several concentration of G-like nucleotides at a central chains. Either PN and LL increase with the concentration of G, i.e., diminishing the degree of disorder. Indeed, for the low disorder case of G corresponding to 95% of the sites, a diffusive regime may be
observed for the present model Hamiltonian. A completely ordered system would imply in transmission probabilities close to the unity, leading to numerically instabilities in defining the LL by means of equation 5. However, the PN can be easily defined for the ordered system and this case is included in figure 5 and it is worth noting that it follows the expected steepness but in the range $L < PN < 2L$, indicating that the LDOS is not evenly distributed among the 4L sites of the system.

5. Conclusions

The present work addresses the question of characterizing the degree of localization in finite disordered systems, considering the case of a more realistic, although heuristic, model for finite DNA-like systems. The degree of localization of electronic states in small systems is relevant in the sense that it could show transport properties of a localized regime in the thermodynamic limit, while a shorter chain could fall within a diffusive regime. This is indeed the case for other models and parametrizations within the same class for which overall longer LL appear [27]. In the present case, a crossover to the $LL > L$ range is only achieved by reducing the degree of disorder. Underneath this potentially interesting possibility of mesoscopic systems, represented here by DNA-like chains, a more fundamental problem has been addressed, namely the behavior of various definitions of localization at lengths below the thermodynamic limit. The present results elucidate the discrepancies among the different definitions of localization at small system sizes, below the thermodynamic limit. These discrepancies can be attributed to the resonances in the system, that play a decreasing role with increasing system length. For the present case, from the point of view of the localization properties, the thermodynamic limit present a threshold in the mesoscopic range, namely at lengths around a few hundreds of nanometers. Finally, having in mind the connection of such heuristic models to real DNA systems, the present results give a simple picture to the great variety among the first experimental results on DNA transport properties [5] realized in the length scales studied here: rather small changes in the degree of disorder, contact strength and electronic structure parameters may considerably modify the transport properties of a modeled device.

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