Absence of extended states in a ladder model of DNA

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According to standard theories of disordered systems, [1] all states in low-dimensional systems with uncorrelated disorder are spatially localized. Therefore, in a pure quantum-mechanical regime, disordered models of DNA might lead to insulator behaviour unless the localization length reaches anomalously large values. To explain long range charge transport found experimentally, [2] several authors considered spatial correlations of the nucleobasis along the DNA molecule. [3–8] Those models are based in the fact that random sequences, having a power-law spectral density $S(k) \sim 1/k^{\alpha}$ with $\alpha > 0$, result in a phase of extended states at the band center, provided α is larger than a critical value α_c. [9–12] As a consequence, long range charge transport might be feasible even at very low temperature, provided the chemical potential lies within the band of extended states.

Recently, Caetano and Schulz claimed that intrinsic DNA-correlations, due to the base pairing (A–T and C–G) between the two strands, lead to electron delocalization even if the sequence of bases along one of the strands is uncorrelated. [13] Furthermore, they pointed out that there is a localization-delocalization transition (LDT) for certain parameters range. If these results were correct, then *transverse* correlations arising intrinsically in DNA could explain long range electronic transport. However, we have claimed that this is not the case and all states remain localized, thus excluding a LDT. [14]

In this work we provides further analytical and numerical support to our above mentioned claim, aiming to understand the role of intrinsic DNA-correlations in electronic transport. To this end, we address signatures of the spatial extend of the electronic states by means of the analysis of the Landauer and Lyapunov coefficients. Thus we introduce the ladder model of DNA [13] and diagnostic tools we use to elucidate the spatial extend of electronic states in the static lattice. Afterwards we discuss the analytical calculation of the Landauer and show that this exponent never vanishes in the thermodinamics limit for any value of the system parameters. From this result we conclude that extended states never arises in the model.

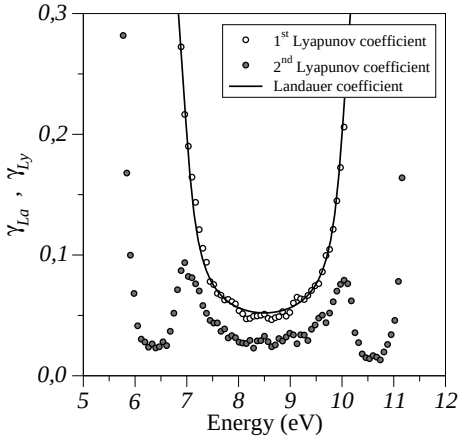

FIG. 1: 2/3 of Landauer exponent γ_{La} (solid line) and the largest Lyapunov exponent γ_{Ly} (white circles), as a function of energy, for $t_{\perp} = 0.5\,\mathrm{eV}$ and $t_{\parallel} = 1.0\,\mathrm{eV}$. The second, smaller Lyapunov exponent (grey circles) is also shown.

We then proceed to calculate the Lyapunov and the Landauer exponent for finite samples for the paramaters used by Caetano and Schulz [13], althoug these values of the interstrand and intrastrand hoppings are larger than those usually considered in the literature, [15, 16]. In Fig.1 it becomes clear that neither the largest Lyapunov exponents nor the Landauer one vanish over the whole energy spectrum. Most important, its minimum value is size independent within the numerical accuracy, suggesting the occurrence of truly localized states. Notice that the minimum value of these exponents is always much larger than the inverse of the number of base pairs ($1/N = 0,00025$), indicating that DNA-pairing can hardly explain long range charge transport at low temperature. From the inverse of the minimum value of the second Lyapunov coefficient we can estimate that the localization length is of the order of 80 base pairs (i.e. roughly eight turns of the double helix), therefore being smaller than typical sizes used in experiments. [2]

To elucidate the effects of the base pairing on the localization length, we have also considered the artificial case of

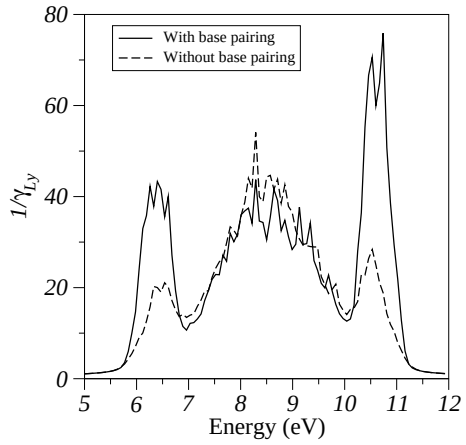

FIG. 2: Inverse of the second Lyapunov coefficient for $N = 4000$ $t_\perp = 0.5\,\text{eV}$ and $t_\parallel = 1.0\,\text{eV}$, when the base pairing is present (solid line) and absent (dashed line)

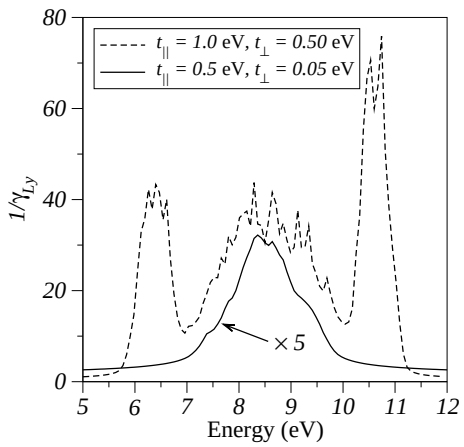

FIG. 3: Inverse of the second Lyapunov coefficient for $N = 4000$ and two sets of hopping parameters, indicated on the legend box. Notice the scaling factor indicated on the lower curve.

ladder models without pairing. Therefore, the system becomes much more disordered and one could naively expect a dramatic decrease of the localization length, as compared to the system with base pairing. Fig.2 indicates that this is not the case. The inverse of the second Lyapunov exponent remains almost unchanged over a large region of the energy spectrum, except close to the two resonances at about 6.4 eV and 10.6 eV. At resonances the localization length is reduced by a factor 2.5 at most when the pairing constraint is relaxed. In any event, resonances still appear so they cannot be associated to base pairing.

Higher hoppings lead to a *less-effective* disorder and higher localization lengths are to be expected. We have calculated the inverse of the second Lyapunov exponent for more realistic values of the hopping parameter and checked that this claim is indeed correct. For instance, for $t_\perp = 0.05\,\text{eV}$ and $t_\parallel = 0.5\,\text{eV}$ (see Ref. 16) the localization length at the center of the band is reduced by a factor 5 as compared to the case shown in Fig.2, while an even larger decrease is noticed at resonances. Therefore, we come to the conclusion that hopping is a more important mechanism for delocalization than base-pairing in this ladder model.

After discussing in detail these exponents' dependence on the model parameters, especially inter- and intrastrand hoppings, we conclude that the localization length is only of the order of very few turns of the double helix for realistic values of the model parameters. Therefore, this shows that intrinsic DNA-correlations alone cannot explain long range electronic transport. found in long DNA molecules. [2]

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