Comment on "Sequencing-Independent Delocalization in a DNA-Like Double Chain with Base Pairing"

In a recent paper [1], Caetano and Schulz (CS) claim that intrinsic DNA-correlations, due to the base pairing (A-T and C-G), lead to electron delocalization. Furthermore, they point out that there is a localization-delocalization transition (LDT) for certain parameter ranges. In this Comment we present analytical and numerical evidences that in their model all states are localized, thus excluding a LDT.

The equation for the electron amplitude can be cast in a compact form by using a 4×4 transfer matrix, $T_{n,ij}$, belonging to the $SU(2, 2)$ group. Here n runs over the sites of one chain and $i, j \in \{\mathrm{A}, \mathrm{T}, \mathrm{G}, \mathrm{C}\}$. Only four different transfer matrices arise ($T_{n,\mathrm{AT}}$, $T_{n,\mathrm{TA}}$, $T_{n,\mathrm{CG}}$, $T_{n,\mathrm{GC}}$).

The Lyapunov exponents, the eigenvalues of the limiting matrix $\lim_{N\to\infty} \ln \prod_{n=N}^{1} T_{n,ij}^{1/N}$, provide information about the localization length of the states, assuming exponential localization. Because of the self-averaging property they can be calculated by taking the product of random transfer matrices over a long system. Similarly, the Landauer exponent $\gamma_{\mathrm{La}}(N) = \ln\langle \| \prod_{n=N}^{1} T_{n,ij} \| \rangle^{1/N}$ ($\langle \ldots \rangle$ denotes ensemble averages) is twice the largest Lyapunov exponent near the critical region in one-dimensional systems [2] and can be calculated analytically following the technique developed in Ref. [3]. For brevity, here we only provide the main steps: We use the decomposition of the product of two fundamental representations, T_n, of the $SU(2, 2)$ group as $(T_n)^{\alpha}_{\alpha'}(T_n^{\dagger})^{\beta'}_{\beta} = (1/4)(\tau^{\mu})^{\beta'}_{\alpha'}\Lambda_n^{\mu\nu}(\tau^{\nu})^{\alpha}_{\beta}$, where τ^{μ} ($\mu = 0, \ldots, 15$) are the generators of the algebra $u(2, 2)$. The matrix $\Lambda_n^{\mu\nu} = (1/4)\,\mathrm{Tr}(T_n \tau^{\mu} T_n^{\dagger} \tau^{\nu})$ is the adjoint representation of T_n. It is then straightforward to get $\langle \Lambda^{\mu\nu} \rangle = (1/4)(\Lambda_{\mathrm{AT}}^{\mu\nu} + \Lambda_{\mathrm{TA}}^{\mu\nu} + \Lambda_{\mathrm{CG}}^{\mu\nu} + \Lambda_{\mathrm{GC}}^{\mu\nu})$. The Landauer exponents are the nonnegative eigenvalues of $\langle \Lambda \rangle$. The condition of the existence of an extended state is equivalent to $\det|\langle \Lambda \rangle - I| = 0$, and it is a matter of simple algebra to prove that this condition is never met.

To provide further support to our claim, we also calculated the localization properties of the system numerically, following the procedure sketched above. The results are collected in Fig. 1 using the same parameters as in Ref. [1]. It becomes clear that neither the largest Lyapunov exponents nor the Landauer one vanish over the whole energy spectrum. Also, the largest Lyapunov exponent for DNA-correlated (with base pairing) and totally uncorrelated (without base pairing) models overlap. In addition, the second, smaller Lyapunov exponent becomes positive too, as seen in Fig. 1 (set labeled B). Most important, its minimal value is size independent within the numerical accuracy (0.0131 ± 0.0035, 0.0124 ± 0.0028, and 0.0127 ± 0.0025 for $N = 2000$, 3000, and 4000, respectively). Therefore, we come to the conclusion that the system studied by CS cannot support extended states. Consequently, a LDT is not to be observed. What is also important, is that lower values of the hopping parameters (in the 1–10 meV range) would result in much less localization length than those obtained by CS. Moreover, some other effects, in particular, polaronic self-trapping due to solvent and counterion dielectric polarization, will further increase the tendency toward charge localization.

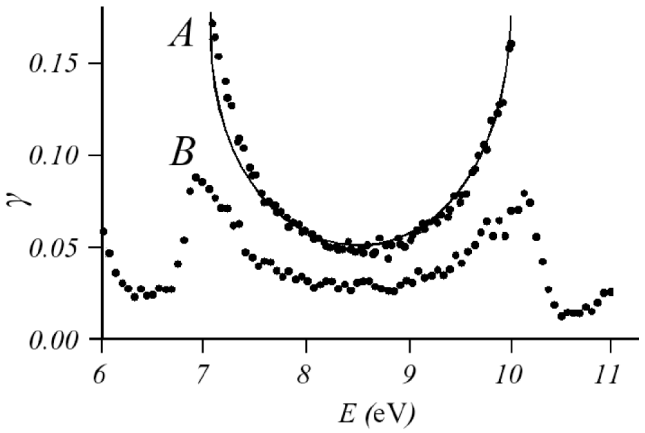

FIG. 1. 2/3 of Landauer exponent γ_{La} (solid line) and largest Lyapunov exponent γ_{Ly}, for both DNA-correlated and totally uncorrelated models, as a function of energy (sets labeled A). Second, smaller Lyapunov exponent (set labeled B).

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