

Multifractal Analysis of a DNA Based Molecular Transistor

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Abstract. The promise of molecular electronics has focused enormous interest on molecular devices. Typically, such devices consist of an individual molecule trapped between two leads, in-between which a voltage bias is applied. Here, we have attempted to design a DNA based molecular transistor. Our aim is choosing the most appropriate parameters such as DNA sequence for creating the most efficient DNA transistor. In this regard, we have used the multifractal analysis to choose the best sequence for electrical transport. The obtained result shows GC rich sequences are the most appropriate sequence. We have studied I-V characteristic diagram for a DNA transistor based on a GC rich sequence. We have observed rectifier behavior of DNA chain via the applied voltage. Negative differential resistance (NDR) is one of the phenomena appears in I-V characteristic diagrams. NDR is applicable in some electrical devices such as electrical switches.

Keywords: DNA based molecular transistor, localization-delocalization transission, Quantum Chaos, Multifractal.

1 Introduction

The programmability, flexibility as well as low cost of synthesis, has made DNA a widely used material for creating the molecular structures and molecular electronics structures such as DNA nanowires, diode or transistor [1]. However, self-assembled DNA-based template nanostructures have been considered as a potential method to create complex three-dimensional electronic circuitry on scales that are not accessible by conventional Silicon based materials [2]. Modern electronics has to face the restrictions dictated by the laws of physics when the minimum feature size of a chip is reduced below a certain length. Designing of any functional electronic device from DNA will require a basic theoretical understanding of how carrier transport actually works in this complex biomolecule [3]. The molecular approach has the interesting advantage of high reproducibility, due to the self-organization and recognition properties of the building blocks (the molecules), and the possibility of implementation of novel functional devices exploiting unusual mechanisms, such as charge transfer, $\pi-\pi$ stack conductivity, molecular rectification, etc [4]. In addition, organic materials require relatively easy and cheap processing technologies for large area and



large scale integration, such as spin-coating and inprint methods.

In this work, we have tried to study the transport properties of a molecular transistor based on organic DNA molecules. We have considered an N-base pairs double-stranded DNA as central molecule and two metal leads with k-sites connected to each strand of DNA. In the complex quantum systems such as mentioned system, one could see critical behaviors such as localization-delocalization transition. The statistical properties of such Hamiltonians coincide with random matrix theory (RMT) emerged from the need to characterize complex quantum systems in which the knowledge of Hamiltonian is minimal. Localization-delocalization transitions of noninteracting electrons are disorder-induced continuous phase transitions. The strong multifractality of wave-function amplitudes of this critical transition is a characteristic feature of transition. The obtained result could be confirmed via the multifractal analysis (MFA) of different sequences. In the following, we have attempted to analyze the transport properties of a DNA transistor based on multifractal analysis.

2 model and method

We have considered a DNA molecule coupled to two Gold leads as a DNA simple DNA transistor. The general Hamiltonian is as following [5,6]

$$H = H_{DNA} + H_{lead} + H_{DNA-lead} \quad (1)$$

The first term describes the double stranded DNA chain as central molecule as following:

$$H_{DNA} = \sum_{j=1,2} \sum_{i=1}^N [(\varepsilon_{j,i} + eV_g) c_{j,i}^\dagger c_{j,i} + t_{i,i+1} c_{j,i}^\dagger c_{j,i+1} + H.c.] + \sum_{i=1} \lambda_i c_{1,i}^\dagger c_{2,i} + H.c. \quad (2)$$

where j and i are number of DNA strands and sites in each strand, respectively. $c_{j,i}^\dagger$ creates an electron at site (j, i) , $\varepsilon_{j,i}$ represents the on-site energy, $t_{j,i}$ is the hopping constant, λ_i is the interchain interaction. Here, V_g is the gate voltage applied for each base of DNA.

H_{lead} represents the left and right contacts in the following form [7]:

$$H_{lead} = \sum_{j=1,2} \sum_k (\varepsilon_{L,j,k} + eV_b/2) a_{L,j,k}^\dagger a_{k,L} + \sum_{j=1,2} \sum_k (\varepsilon_{R,j,k} - eV_b/2) a_{R,j,k}^\dagger a_{k,R} \quad (3)$$

where $a_{\beta,j,k}^\dagger$ with $\beta = L, R$ is the creation operator of an electron in the lead β , $\varepsilon_{\beta,j,k}$ is the on-site energy of leads and V_b is bias voltage.

The final term of Hamiltonian provides the interaction between the DNA chain and leads:

$$H_{DNA-lead} = \sum_{j=1,2} \sum_k (t_L a_{L,j,k}^\dagger c_{j,1} + t_R a_{R,j,k}^\dagger c_{j,N} + H.c.) \quad (4)$$

where t_β is tunneling matrix elements from a site k of the lead β to the DNA chain.

We have considered an N base pairs double-stranded DNA as central molecule and two metal leads with k sites connected to each strand of DNA. Hamiltonian matrix corresponding to the current model would be a $(2N + 4k) \times (2N + 4k)$ matrix. In the complex quantum systems such as our Hamiltonian, one could see critical behaviors such as localization–delocalization transition. The statistical properties of such Hamiltonians coincide with random matrix theory (RMT) emerged from the need to characterize complex quantum systems in which the knowledge of Hamiltonian is minimal [8].

Thus, we expect underlying ideas to radiate beyond spectral fluctuations, such as transport and localization. In this regard, we have studied the system using the multifractal analysis.

2.1 Multifractal analysis

Localization–delocalization transitions of noninteracting electrons are disorder-induced continuous phase transitions [9]. The strong multifractality of wave-function amplitudes of this critical transition is a characteristic feature of transition [10]. Wave functions (WFs) are neither localized nor simply extended, but are complicated scale invariant fractals at the transition point that exhibits multifractal behavior characterized by a continuous set of scaling exponents [11,12]. The multifractality of the eigenstates is characterized by its associated singularity spectrum $f(\alpha)$. The q th moments of the inverse participation ratio P_q , defining the scaling behavior of P_q with length λ , can be applied for the computation of $f(\alpha)$. Considering $|\Psi|^2$ as the normalized electronic wave function of the i -th site in a discretized d -dimensional system with volume L^d , one can compute the probability of finding the electron in the k th box by covering the system volume with N_l boxes of linear size l . So

$$\mu_k(l) = \sum_{i=1}^{l^d} |\Psi_i|^2, \quad k = 1, \dots, N_l \quad (5)$$

The $\mu_k(l)$ constitutes a normalized measure for which we can define the q th moment as

$$P_q(l) = \sum_{k=1}^{N_l} \mu_k^q(l) \quad (6)$$

The general assumption underlying multifractality is that moments P_q show a power-law behavior that indicates the absence of length scales in the system. within a certain range of values for the ratio,

$$P_q(\lambda) \propto \lambda^{\tau_q} \quad (7)$$

Where, λ is defined as $\lambda \equiv l/L$. The mass exponent τ_q is defined as

$$\tau(q) = \begin{cases} d(q-1) & \text{for metals} \\ 0 & \text{for insulators} \\ D_q(q-1) & \text{at the MIT} \end{cases} \quad (8)$$

where D_q are the generalized fractal dimensions. A Legendre transformation can be resulted in singularity spectrum f_α is obtained from the τ_q exponents via,

$$f(\alpha_q) = \alpha q - \tau(q) \quad (9)$$

Here, f_α holds for the fractal dimension of the set of points where the wave-function intensity is $|\Psi_i|^2$, which is in discrete systems the number of such points N_α scaled as $L^{f(\alpha)}$. The singularity spectrum $f(\alpha)$ is a convex function of α , and its maximum value occurs at α_0 , with $f(\alpha_0) = d$.

The larger the value of i_{scale} is, the more non-periodic the signal is. Narrower diagrams of $f(\alpha)$ corresponds with more delocalized states, such that in the case of fully delocalized state the singularity spectrum converges to one point $f(d) = d$. On the other hand, as the system undergoes a localization transition the singularity spectrum broadens. This feature aids us to distinguish localized states from delocalized ones. As a result, only at MIT the system can show multifractal behavior. In recent decades, MFA of electronic wave function at localization-delocalization transition has been a hot topic for study [13,14]. Therefore, we have attempted to use the multifractal analysis for distinguishing between the different transport states in DNA transistor.

The complex structure of DNA complicates the experimental measurements of conductivity [15,16]. The *GC* content of DNA appears to strongly influence the electrical properties of DNA. DNA behaves as a broad band-gap semiconductor that which band gap energy decreases with the increasing number of *GC* bases. This role of the *GC* is based on the fact that guanine has the lowest electrochemical potential of all bases and therefore facilitates charge transfer along the DNA observed previously [17].

We have considered $f(\alpha)$ for different DNA sequences with different *GC* richness and $N = 1000$ base pairs (Fig. 1). For the DNA chain, $\varepsilon_{j,i}$ is chosen with $\varepsilon_A = 8.5$, $\varepsilon_C = 8.9$, $\varepsilon_G = 8.3$, $\varepsilon_T = 9$ eV. The tunneling elements between identical neighboring bases ($t_{j,i}$) are taken as $t_{AA} = 0.22$, $t_{TT} = -0.14$, $t_{CC} = -0.05$, $t_{GG} = 0.11$ and $\lambda_i = -0.3$ with the units in eV [18–20]. $t_{j,i}$ between different neighboring bases X and Y is set to $t_{XY} = (t_{XX} + t_{YY})/2$, in accordance with first-principle results [21]. Also, $\varepsilon_{\beta_{j,k}} = 7.75$ eV and $t_\beta = 0.42$ eV are the parameters [22]. It is appeared that a *GC* rich sequence shows the delocalized state as a result of the nearly conductive behavior. It is clear that all of them show a concave behavior. If we consider the wider interval for α parameter, it could be seen that the diagrams are smooth and they behave closer to conductivity state. These sequences with good conductivity could be the appropriate candidate in molecular transistor applications. If we increase *AT* content of the sequence, we would approach to the critical behavior. One could see a critical *AT* content of the DNA sequence where in this value, DNA shows a critical behavior. This behavior confirms a metal–insulator transition. Via the increasing the percentage of the *AT* and hence decreasing the *CG* content of sequence, $f(\alpha)$ graphs go to be flatter. This manner corresponds to localized manner.

Therefore, one can observe that the appropriate sequence for using in DNA transistor is the richest *GC* content, where, $f(\alpha)$ is flatter than others.

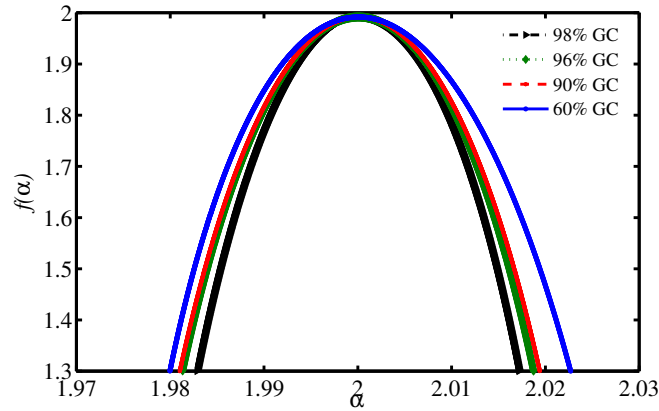


Fig. 1. Multifractal spectrum for different sequences.

2.2 I-V Characteristic diagram

It is worth mentioning that one of the characteristic properties of a electronic device is its I-V characteristic diagram. I-V characteristic diagram determines the transport properties of system in different applied potentials. Figure 2 shows variation of the electrical current flowing through the DNA channel with respect to the bias voltage. Here, DNA transistor acts with the most appropriate sequence for transport. It is clear that channel shows a rectifier behavior. It means that changing the applied voltage direction change the electrical current generally. Also, one can observe Negative differential resistance (NDR) phenomenon in the current flowing through DNA. It means that increasing the applied potential corresponds to decreasing the current [23,24]. NDR has been attributed mostly to resonant tunneling between molecular orbitals and the metal delocalized states [25]. This phenomenon was previously observed in DNA. On the other hand, we have examined the effect of gate voltage on the transport properties of transport (Fig. 3). Diagram shows that increasing the gate voltage corresponds to the current amplification through the transistor. The rectifier behavior of channel versus the gate voltage is clear. Also, one can report that the response of transport channel with respect to applied gate voltage is as an NDR behavior.

3 Conclusion

To meet the future trend as well as the need for smart, wearable, and foldable devices, organic-based electronics, such transistors and so on, have attracted much attention in recent years. Organic molecular transistors are considered as a key component of nanoscale integrated circuits for use in flexible smart cards, low cost radio frequency identification (RFID) tags, and organic active matrix. In the current study, we have attempted to determine most appropriate situation for engineering a DNA based transistor. In this regard, we have used

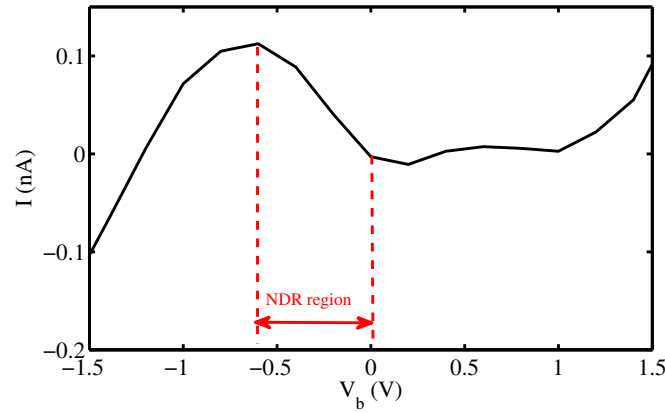


Fig. 2. Electrical current flowing through the DNA channel in different bias voltages.

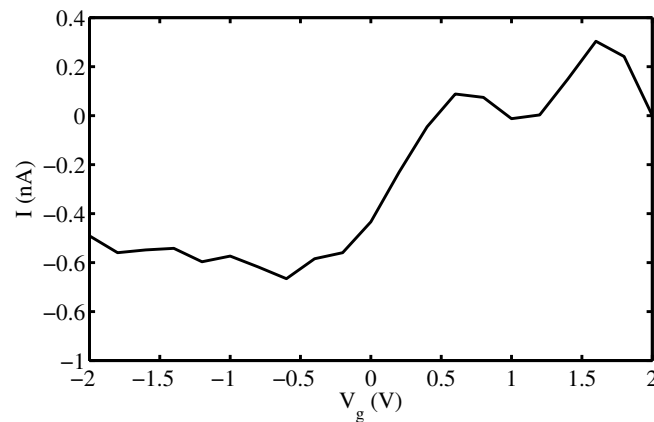


Fig. 3. Electrical current flowing through the DNA channel in different gate voltages.

the multifractal analysis to choose the suitable DNA sequence. It shown that the CG rich sequences are better than other sequence for transport. Therefore, we have chosen a GC rich sequence as a conductivity channel in DNA transistor and studied its transport properties as I-V characteristic diagram. The obtained results shows NDR behaviour and rectifier property of channel. NDR is an effective phenomenon in designing the electronically switches. displays

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