

## Engineering of a Temperature Dependent Thermal Bath Coupled to a Biosystem

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**Abstract.** In the emerging field of nanoelectronics, biosystems have drawn in the past decade the attention of both experimentalists and theoreticians. Flexibility, programmability, and not expensive synthesis of biosystems make them the appropriate candidate for nanoelectronic applications. Biosystems can show different electrical properties. Therefore, the identification of the relevant charge transport channels in biosystems becomes a crucial issue. In the current study, the electronic transport through a biosystem in the presence of the environment is investigated. We obtain the eigenvalues and eigenstates of the Hamiltonian matrix. Analyze is based on the statistical distribution of the energy levels. We have varied the system parameters and investigate the stability properties of system. Total spin current ( $S_t = S^\uparrow + S^\downarrow$ ) in short sequences shows the localization behavior and by increasing length of sequences we can see nearly extended state, delocalization and more spin current.

**Keywords:** Quantum chaos tools, Nanoelectronic, Heat bath, Biosystem.

### 1 Introduction

In recent years, the syllable “bio” has become a powerful attribute to attract public attention for designated “green” processes. “Bio” is generally used in a broad context which often complicates communication between experts and beginners in this interesting field. Often they are denoted as biomaterials, but this term is also widely used for any interaction between biological and non-biological systems. Biology and electronics are both expert at for accessing, analyzing, and responding to information. Biology uses ions, small molecules, and macromolecules to receive, analyze, store, and transmit information, whereas electronic devices receive input in the form of electromagnetic

radiation, process the information using electrons, and then transmit output as electromagnetic waves [1]. One of the most decisive properties of organic electronics to successfully enter the future market is their inherent flexibility due to the weak intermolecular forces of organic semiconductors [2]. Biomolecules often have natural electrical and optical properties that are fine-tuned to improve device performance. The main goal in biosystems is enhancing the performance, naturally occurring biomolecules also support renewable and environmentally responsible electronics, with the potential of a concomitant reduction in cost [3]. The study of functioning of biological systems is due to the microscopic dimension of systems, under the knowledge of quantum biology. This field of science refers to applications of quantum mechanics and theoretical chemistry for biological fields [4].

Modern research activities, both theoretical and experimental, inevitably deal with open quantum systems such as quantum transport through molecular wires and mesoscopic devices, biological or artificial light-harvesting complexes, controlling quantum entanglement in realistic spins and/or photonic devices, quantum measurement and quantum information [5]. Among the biological systems, the DNA molecule has special attention due to its unique properties. Physicists are more and more interested in 'complex systems' where the interplay of many individual components leads to new phenomena. Biological molecules provide fascinating examples of such complex systems and this is why they are attracting the attention of a growing number of physicists. From the point of view of a physicist the DNA molecule is only a system consisting of many interacting atoms organized in a special way in space. The programmability, flexibility, as well as low cost of synthesis have made DNA a widely used material for creating molecular structures and molecular electronics structures such as DNA nanowires, diodes, or transistors [6]. There has also been increasing interest in the potential of the DNA molecule for constructing of nanostructures of high complexity, as well as the design of nanoelectronic devices, nanosensors, and nanocircuits (all of them rely on its electronic properties) [7,8]. Theoretical understanding of the carrier transport mechanism is the main constituent of designing the DNA-based functional electronic device. The development of structural DNA nanotechnology relies on the control of the transport properties of DNA also thermal fluctuations and environment effects play a major role in DNA functioning. We have considered the molecule as being static. This approach has been widely used in the study of the DNA structure but, in reality, the DNA molecule is usually immersed in some thermal bath and environmental conditions, and its structural elements such as individual atoms, groups of atoms (bases, sugar rings, phosphates), fragments of the double chain including several base pairs, are in constant motion, and this motion plays an important role in the function of the molecule [9].

In current study, we try to unveil the spin transport properties of a DNA-based molecular system. The spin-selectivity features of DNA molecules have provided promise for chiral molecule-based spintronic devices where the spin

degree of freedom can be manipulated for practical applications [10-12]. To this aim, we coupled double-strand-DNA (dsDNA) molecules to two leads in the chain ends and to a thermal bath. The bath consists of a collection of weakly-interacting components (“molecules”), each having finitely-many degrees of freedom. The thermal bath can play the role of the environment effects for the system. Using the natural sequence of the dsDNA molecule or human chromosome 22 (Ch22), some properties of systems is investigated like symmetry failure, localization decreasing and extended spin distribution via the increasing the sequence length and voltage change by using quantum chaos tools.

## 2 Model

We have considered a DNA molecule coupled to two leads embedded in thermal bath. As show in figure 1, the general Hamiltonian is as following [6]:

$$H_{SYS} = H_{DNA} + H_{Lead} + H_{Bath} + H_{DNA-Lead} + H_{DNA-Bath} \quad (1)$$

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

$$\begin{aligned} H_{DNA} = & \sum_{i,j=1,2} \sum_{\sigma=\uparrow\downarrow} \varepsilon_{i,j} c_{i,j}^{+\sigma} c_{i,j}^{\sigma} + V_{i,i+1,j} c_{i+1,j}^{+\sigma} c_{i,j}^{\sigma} + \sum_{i,\sigma} \lambda_i c_{1,i}^{+\sigma} c_{2,i}^{\sigma} \\ & + \sum_{i,j} 2it_{so} \cos\theta (c_{i,j}^{+\uparrow} c_{i+1,j}^{\uparrow} - c_{i,j}^{+\uparrow} c_{i-1,j}^{\uparrow} - c_{i,j}^{+\downarrow} c_{i+1,j}^{\downarrow} + c_{i,j}^{+\downarrow} c_{i-1,j}^{\downarrow} \\ & + D_{i,i+1} c_{i,j}^{+\uparrow} c_{i+1,j}^{\downarrow} - D_{i,i+1}^* c_{i,j}^{*\downarrow} c_{i+1,j}^{\uparrow} + D_{i-1,i}^* c_{i,j}^{+\downarrow} c_{i-1,j}^{\uparrow} - D_{i-1,i} c_{i,j}^{+\uparrow} c_{i-1,j}^{\downarrow}) + H.c. \end{aligned} \quad (2)$$

Where  $j, i$  and are number of DNA strands and sites in each strand, respectively.  $c_{i,j}^{+}$  creates an electron at site  $(i, j)$ ,  $\varepsilon_{i,j}$  represents the on-site energy,  $\lambda_i$  is the interchain interaction.  $t_{so}$  represents the spin-orbit coupling constant.

$D_{n,n+1} = it_{so} \sin\theta \{ \sin[n\Delta\phi] + \sin[(n+1)\Delta\phi] + i \cos[n\Delta\phi] + i \cos[(n+1)\Delta\phi] \}$   
That  $\theta$  is the helix angle and  $\phi = n\Delta\phi$  is the cylindrical coordinate with  $\phi$  the twist angle. Preservation of time reversal symmetry leads to  $D_{n,n-1} = D_{n-1,n}^*$ .  
Second term represents the left and right lead contacts in the following form [13]:

$$H_{Lead} = \sum_{j=1,2} \sum_{k,\sigma} (\varepsilon_{L,j,k} + \frac{eV_b}{2}) a_{L,j,k}^{+\sigma} a_{L,j,k} + \sum_{j=1,2} \sum_{k,\sigma} (\varepsilon_{R,j,k} - \frac{eV_b}{2}) a_{R,j,k}^{+\sigma} a_{R,j,k} \quad (3)$$

Where  $a_{\beta,j,k}^{+}$  ( $a_{\beta,j,k}$ ) with  $\beta = L, R$  is the creation (annihilation) operator of an electron in the lead  $\beta$ ,  $\varepsilon_{\beta,j,k}$  is the on-site energy and  $V_b$  is bias voltage.  $H_{bath}$  is

the Hamiltonian of the oscillators chain which arises from a nearest neighbor Hook-like coupling model [14]:

$$H_{Bath} = \sum_{i=1}^N \hbar \omega_i b_i^\dagger b_i + 2 \sum_{i=1}^{N-1} \hbar \Omega_i (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + H.c. \quad (4)$$

where  $b_i^\dagger$  is the creation operator of an oscillation in the  $i$ -th oscillator and  $\omega$  and  $\Omega$  are the oscillator frequency and their mutual coupling constants, respectively. The fourth term of the Hamiltonian provides a DNA-lead tunneling as follows [15]:

$$H_{DNA-Lead} = \sum_{j=1,2k,\sigma=\uparrow\downarrow} \sum (t_L a_{L,j,k}^{+\sigma} c_{i,j}^\sigma + t_R a_{R,j,k}^{+\sigma} c_{j,N}^\sigma + H.c.) \quad (5)$$

where  $t_\beta$  is the tunneling matrix element from the lead  $\beta$  to the DNA chain. The final term describe interaction between DNA and bath:

$$H_{DNA-Bath} = \sum_{i=1}^N \sum_{\sigma=\uparrow\downarrow} \sum_{j=1,2} t_i b_i^\dagger c_{i,j}^\sigma + H.c. \quad (6)$$

where  $t_i$  is the interaction constant.

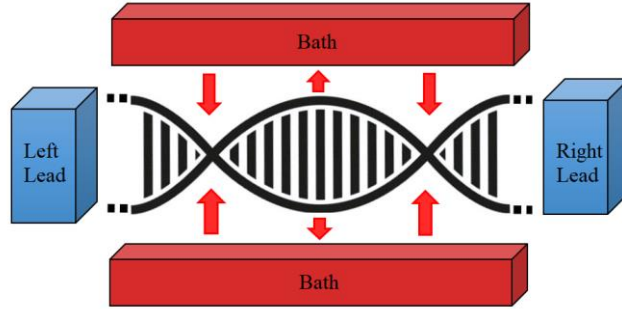


Fig. 1. Scheme of a chiral DNA molecule sandwiched between leads and embedded in the heat bath

### 3 Methods

We have considered an  $N$  base pairs dsDNA as central molecule which each strand is connected to an  $N$  site thermal bath and double-stranded metal leads

with  $k$  sites in two chain ends. The Hamiltonian matrix corresponding to the current model would be a  $(6N + 8k) \times (6N + 8k)$  matrix.

The spectral fluctuations of such a matrix could be analyzed through the probability distribution of the nearest neighbor level spacings  $P(s)$ .  $P(s)$  is one of the most applied tools in the study of spectral correlations where the nearest-neighbor spacing is calculated as  $s = E_{i+1} - E_i$ . In the regular spectrum, the distribution of energy eigenvalues is random where spacing between adjacent levels is distributed as Poissonian [15] and corresponds to a localized phase. The fluctuations of quantal spectra with irregular behavior reveal a Gaussian distribution. It is said that the states of diffusive metal exhibit Wigner-Dyson level statistics [17] and show that system has delocalize behaviour.

By using Inverse participation ratio (IPR) we can study the localization properties of a system. Inverse participation ratio (IPR) defined as [18]:

$$IPR(E_\alpha) = \sum_i |\psi_i^\alpha|^4 \quad (7)$$

where  $\psi_i^\alpha$  is the amplitude of the eigenstate with energy  $E_\alpha$  on site  $i$ . We expect that  $IPR = 1$  for a completely localized state, and  $IPR = 1/\dim(H)$  for a fully extended state. The complementary information about the dynamics of a spectral fluctuation could be provided via the  $IPR$  dynamics. A Hamiltonian system in contact of heat baths with a friction and a thermal drive feature plays as a dissipative system. It is the outstanding property of the nonlinear systems that small variation in a parameter can lead to abrupt changes in both the quantitative and qualitative behaviour of the system (chaotic systems).

Localization-delocalization transitions of noninteracting electrons are disorder- induced continuous phase transitions. This critical transition has strong multifractality of wave- function amplitudes and is a characteristic feature of transition. The multifractality of the eigenstates is characterized by its associated singularity spectrum  $f(\alpha)$ . 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  $l$ .

$$\mu_k(l) = \sum_{i=1}^{l^d} |\psi_i|^2, \quad k = 1, \dots, N_l \quad (8)$$

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

$$P_q(l) = \sum_{k=1}^{N_l} \mu_k^q(l) \quad (9)$$

Within a certain range of values for the ratio,  $P_q(\lambda) \propto \lambda^{\tau_q}$  where  $\lambda$  is defined as  $\lambda \equiv l/L$ . The mass exponent  $\tau_q$  is defined as

$$\tau_q = \begin{cases} d(q-1) & \text{for metals} \\ 0 & \text{for insulators} \\ D_q(q-1) & \text{for MIT} \end{cases} \quad (9)$$

where  $D_q$  are the generalized fractal dimensions. A Legendre transformation can be resulted in singularity spectrum  $f(\alpha)$  is obtained from the  $\tau_q$  exponents via,

$$f(\alpha_q) = \alpha q - \tau(q) \quad (10)$$

The singularity spectrum  $f(\alpha)$  is a convex function of  $\alpha$ , and its maximum value occurs at  $\alpha_0$ , with  $f(\alpha_0) = d$ . In this study  $d = 2$  which equal to dimensional system.

## 4 Results

The aim of the current study is investigation of spin current in different condition in a bio-molecular devices based on a DNA bridge between the metal electrodes. The DNA ability for long-range charge transport has become a challenging debate, due to the envisioned impact of charge transport in molecular (bio) electronics [19]. We consider the effect of environment as well as DNA chain sequence on the incorporation of DNA molecules into electronic devices and circuits. Here, we choose  $\varepsilon_A = 8.5$ ,  $\varepsilon_C = 8.9$ ,  $\varepsilon_G = 8.3$  and  $\varepsilon_T = 9eV$  for  $\varepsilon_{i,j}$  values. On the other hand,  $t_{AA} = 0.22$ ,  $t_{TT} = -0.14$ ,  $t_{CC} = -0.05$ , and  $t_{GG} = -0.11$  are the tunneling elements between the identical neighboring bases and  $\lambda_i = -0.3$  [6].  $t_{i,j}$  between different neighboring bases  $X$  and  $Y$  is calculate by  $t_{XY} = (t_{XX} + t_{YY})/2$ . Also,  $\varepsilon_{\beta_{j,k}} = 7.75eV$  and  $t_\beta = 0.42eV$  are the lead parameters [20]. The bath frequency is  $\omega/\omega_c = 5$  in which  $\omega/\omega_c = \gamma T$  with  $T = 300K$  and  $\gamma$  is the constant of proportionality.

### 4.1 Nearest neighbor level spacings $P(s)$

The diagrams of  $P(s)$  show different behavior for each of the sequences. Fig.2 shows the nearest neighbor level spacing for 200bp DNA sequence. The primary peak in fig.2 is known as Shnirelman peak [21]. In fig.3 nearest

neighbor level spacing is show for 1000bp DNA. The primary peak is decreasing and  $P(s)$  comes closer to the Poisson diagram.

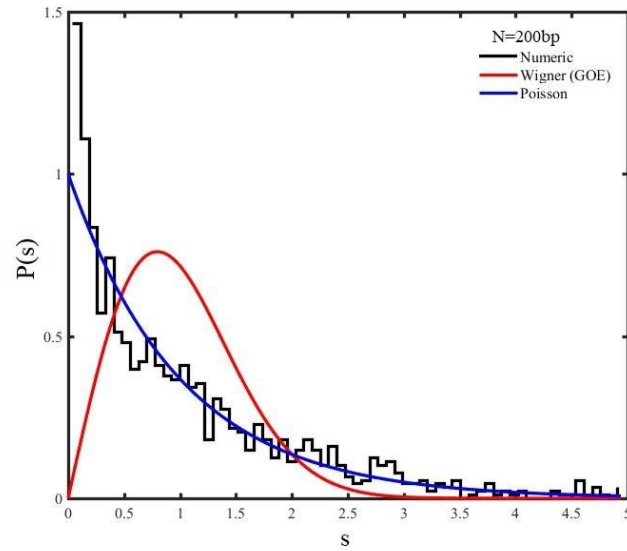


Fig. 2. Nearest-neighbor level distribution for ch22-200bp

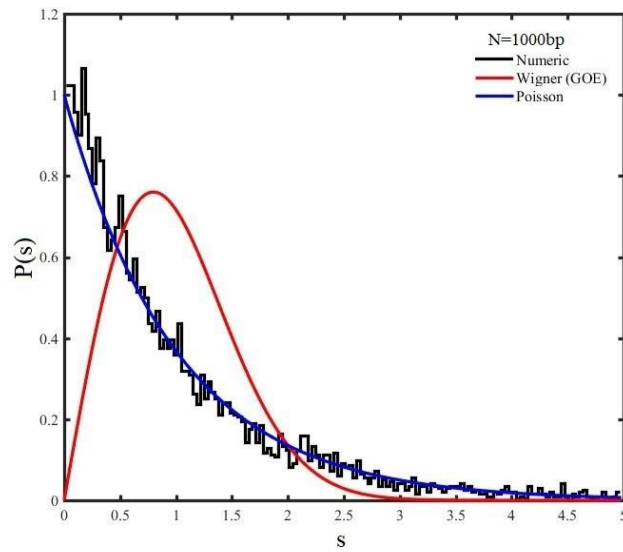


Fig. 3. Nearest-neighbor level distribution for ch22-1000bp

#### 4.2 Inverse participation ratio (IPR)

In this analysis,  $IPR = 1$  means that the system is in a localized regime and for  $IPR = 1/\dim(H)$  means that the system is in a fully delocalized regime. According to the values obtained in the table 1, the system show localize behavior and localization in wave function. Based on this analysis the system localization decrease by increasing the length of base pairs.

Length of sequences	$IPR$
60 bp	0.0854094
200 bp	0.0714314
500 bp	0.0562663
1000 bp	0.0412777

Table 1. IPR values for different sequences of DNA

#### 4.3 Multifractal analysis $f(\alpha)$

Fig.4 determines  $f(\alpha)$  for four different sequence. For short length DNAs, the  $f(\alpha)$  go to be flatter and by increasing the length of sequence the width of  $f(\alpha)$  decreases. The less width of graphs corresponding to extended states and the flatter graphs means localization states. The extended wave function means that by increasing length of sequence some of the system symmetries is broken.



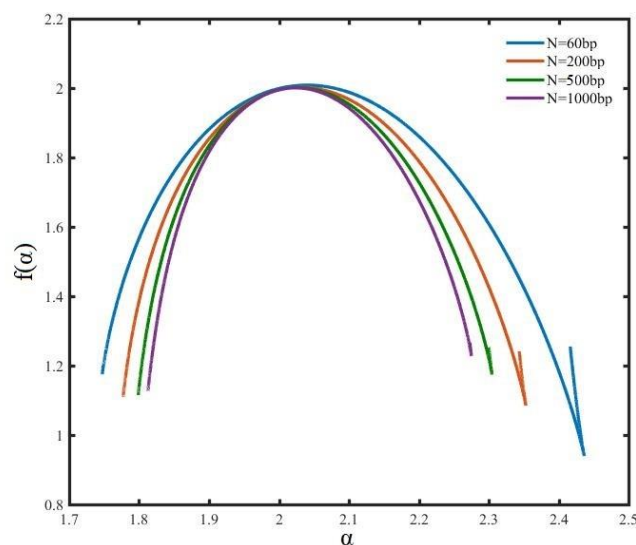


Fig. 4. Multifractal analyses for different sequences of DNA

## Conclusions

In current study, to simulation the environmental effects on the molecules, we contact the molecules with the electrodes and sandwiched in thermal bath. Temperature, ambient frequency and length of sequences are the key parameters for many crucial biochemical reactions in biological system. We have analyzed a biological system with DNA natural sequence of ch22 as a central molecule by using the Quantum Chaos tools. In addition, we have investigated the spin propagation and localization for different sequences by applying different voltage through the electrodes. Total spin current ( $S_t = S^\uparrow + S^\downarrow$ ) in short sequences shows the localization behavior and by increasing length of sequences we can see nearly extended state, delocalization and more spin current. The obtained results demonstrated the symmetry failure, localization decreasing and extended spin distribution via the increasing the sequence length.

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