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Transport Properties of a DNA Transistor in the Presence of a Thermal Bath

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Abstract. DNA nanotechnology is a purist's approach to biomolecular engineering. The field aims to create molecular structures and devices through the exclusive use of DNA as an engineering material. On the other hand, creating of a molecular transistor as well as engineering its structure have become one of the greatest aims of scientists. We have focused on the environmental dependent behavior of a DNA-templated transistor. Our aim is choose the most appropriate parameters for designing the DNA transistor. The bath parameter strongly affects on transfer properties of a DNA transistor. But, the results have shown that the sequence content in the presence of the bath have lower impact than the bath parameters while it is very important factor in absence of bath. As it is shown, it is possible that via the adjustment of bath parameters, one designs a conductivity channel for all nucleotide contents. Thus, one can engineer a DNA based transistor simply through the setting of only one parameter.
Keywords: DNA nanoelectronics, molecular transistor, thermal bath, nearest neighbor level distribution.

1 Introduction

To meet the future trend as well as the need for smart, wearable, and foldable devices, organic-based electronics, such as display [1-3] sensors [4-5], transistors and so on, have attracted much attention in recent years. Flexible electronic circuits are an essential prerequisite for the development of rollable displays, conformable sensors, biodegradable electronics and other applications with unconventional form factors [6]. Organic transistors have attracted interest in areas of chemistry, physics, materials, and nanoelectronics [7, 8]. On the technological side, 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 displays [9, 10]. In order to obtain transistors with high performance, a large amount of effort has been devoted to the synthesis of novel semiconductors and the development of new fabrication techniques [11, 12]. In this regard, molecular transistors which is made of a nanoscale molecular channel material and flow of electrons is controlled by modulating the energy of the molecular orbitals, has attracted considerable attention in recent years primarily for their potential applications in nano-technology. A molecular transistor is an electronic device in which a central molecule connected by metal leads (source and drain), plays the important role in transport. Is it possible that DNA plays a

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role of molecular transistor in a nanoelectronic circuit? Exceptional properties of the DNA molecule including the conductivity properties has made DNA molecule as a promising candidate for molecule electronic devices [13, 14]. The DNA ingredients and environmental effects such as temperature, humidity, solvent, ions, substrate and external fields can affect the conductivity properties of DNA. Therefore, designing the functional circuits from DNA will require at least a basic theoretical understanding of carriers transport in this complex biomolecule [15]. In this work, we have tried to study the transport properties of a molecular transistor based on DNA molecules in environmental conditions. This made it possible to design an environment dependent molecular transistor. Here, DNA chain as a central molecule is attached to the two metals leads and is in the contact of the thermal bath. The goal is developing the new method based on quantum behavior of charge transfer in DNA transistor. We have chosen quantum chaos tools for studying the transport properties of our system. Therefore, we want to use from this fact that each completely hyperbolic classical dynamics has a quantum energy spectrum with the same fluctuations as a random matrix caricature [16]. In this work, we have tried to investigate the requirements for achieving to a high performance DNA based transistor in the contact of a thermal bath. We have used the nearest neighbor level distribution for determining the affected factors on the transport properties of transistor.

2 Materials and method

We have started from a Hamiltonian model for a DNA molecule coupled to two leads and is in the contact of a thermal bath. The mentioned Hamiltonian is as following:

$$H = H_{DNA} + H_{Lead} + H_{DNA-Lead} + H_{Bath} + H_{DNA-Bath} \tag{1}$$

where H_{DNA} describes the isolated double stranded DNA chain as a central molecule through the following approach [17]:

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

where $c_n^{+}(c_n)$ is creation (annihilation) operator for an electron at site i, j. $\varepsilon_{i,j}$ represents the on-site energy, $i, i+1$ is hopping integral and V_g is the gate voltage.

Left and right contacts are specified as following [18]:

$$H_{Lead} = \sum_{k} \sum_{j=1,2} (\varepsilon_{L_{k,j}} + \frac{eV_b}{2}) a_{L_{k,j}}^{+} a_{L_{k,j}} + (\varepsilon_{R_{k,j}} - \frac{eV_b}{2}) a_{R_{k,j}}^{+} a_{R_{k,j}} \tag{3}$$

where $a_{\beta_{k,j}}^{+} (a_{\beta_{k,j}})$ $(\beta = L, R)$ is the creation (annihilation) operators of an electron in the lead β, $\varepsilon_{\beta_{k,j}}$ is the on-site energy and V_b is bias voltage.

The third term of Hamiltonian provides an electron-phonon tunneling via the DNA-lead connection as follows [18]:

$$H_{DNA-Lead} = \sum_k \sum_{j=1,2} t_L a_{L_{k,j}} c_{1,j} + t_R a_{R_{k,j}} c_{N,j} + H.c. \tag{4}$$

where t_β is tunneling constant from the lead β to the DNA.

Hamiltonian of the oscillator's chain arises from following Hamiltonian [19]:

$$H_{Bath} = \sum_{i=1}^{N} \hbar\omega_i b_i^+ b_i + 2\sum_{i=1}^{N} \hbar\Omega_i (b_i^+ b_{i+1} + b_{i+1}^+ b_i) \tag{5}$$

where b_i^+ is the creation operator of an oscillation in $i-$th oscillator, ω_i and Ω_i are the oscillator frequency and their mutual coupling constants, respectively.

Coupling of the Bath and DNA lattice considered as:

$$H_{transistor-Bath} = \sum_{i=1}^{N} t_i b_i^+ c_i + H.c. \tag{6}$$

in which t_i is the interaction constant. The bath can be described by a spectral density as:

$$J(\omega) = \sum_i t_i^2 \delta(\omega - \omega_i) = J_\circ (\frac{\omega}{\omega_c}) e^{-\frac{\omega}{\omega_c}} \Theta(\omega) \tag{7}$$

that ω_c is a cut–off frequency and $\Theta(\omega)$ is the Heaviside function.

The Hamiltonian matrix corresponding to the current model would be a $(4N+4k)\times(4N+4k)$ matrix. The spectral fluctuations of such a matrix could be analyzed through the probability distribution of the nearest neighbor level spacings $(P(s))$. It is worth mentioning that the fluctuations of quantal spectra with irregular behavior reveal Gaussian distribution. It is said that the states of diffusive metal exhibit Wigner-Dyson level statistics [20]. On the other hand, the distribution of energy eigenvalues is random where spacing between adjacent levels distributed as Poissonian [21]. Near a mobility edge, extended states show quantum critical scaling in the overlap of wave-function probabilities at different energies [22].

We have studied the energy levels statistics in our DNA based system using the full Hamiltonian model. The parameters used in this study are as following: For DNA chain, $\varepsilon_{j,i}$ are chosen as $\varepsilon_A = 8.5,\ \varepsilon_C = 8.9,\ \varepsilon_G = 8.3,\ \varepsilon_T = 9\ eV$. The tunneling constants between the same base-pairs are $t_{AA} = 0.22,\ t_{TT} = -0.14,\ t_{CC} = -0.05,\ t_{GG} = 0.11,\ \lambda_i = -0.3\ eV$. On the other hand, t_{ji} between the different base-pairs are $t_{XY} = \frac{t_{XX} + t_{YY}}{2}$ and the lead parameters are $\varepsilon_{\beta_{j,k}} = 7.75\ eV$ and $t_\beta = 0.42\ eV$.

3 Results and Discussion

The aim of the current study is designing a nanoscale, flexible and high performance transistor based on DNA chain bridged between two metal electrodes. We elaborate on the role played by the environment by addressing signatures of the bath on charge transfer of DNA channel. Therefore, we have examined the effect of bath parameters on localization/delocalization process in DNA. Figures 1-3 shows the effect of bath parameters $J_{\circ}/\omega_c$ on the nearest neighbor level distribution. Here, we have tried to study the different states of the DNA channel via the variation of bath frequencies. This work is done for a fixed DNA sequence (100% CG content). We have varied $J_{\circ}/\omega_c$ parameter from 1 to 30. Figure 1 shows $P(s)$ for $J_{\circ}/\omega_c = 1$. It is clear that for this value, system shows a Poissonian and then, localized state for electron transferred through the channel. By increasing $J_{\circ}/\omega_c$ parameter up to 4, system starts to go to a transition state. In this situation, system gradually tends to delocalised behaviour (Fig. 2). $P(s)$ diagram for such values is not Poisson nor Wignerian. It is a critical behaviour for our transport channel. We have continued this work for bath parameter up to 40 (Fig. 3). The obtained results show that for all parameter values up to 30, system behaves as a semi conductive channel. It is desirable situation for designing a Conductive channel for current transfer in transistor. It is in agreement with recent studies on electronic conductivity properties of DNA have reported the emergence of delocalized states as a result of the base pairing of DNA [23].

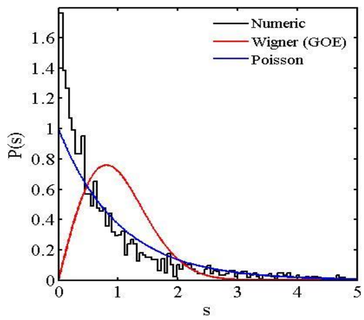

Fig. 1. Nearest neighbor level distribution for $J_{\circ}/\omega_c = 1$.

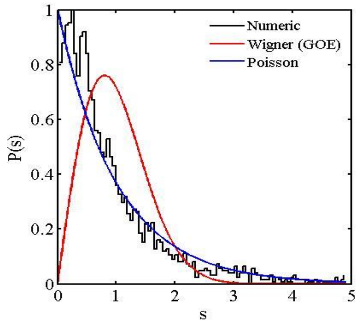

Fig. 2. Nearest neighbor level distribution for $J_{\circ}/\omega_c = 4$.

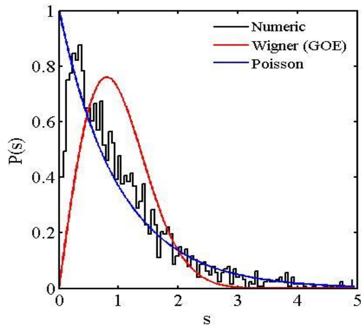

Fig. 3. Nearest neighbor level distribution for $J_{\circ}/\omega_c = 30$.

We know that the nucleotide chain of DNA is an intrinsic disorder property in the DNA molecule against the charge transfer [24]. Therefore, the extent and efficiency of charge transfer is discussed as a function of sequence dependent energetics. It was shown that the DNA molecule with different sequences could present any transport behavior: conducting, semiconducting, and insulating48 and even to be a proximity induced superconductor [25-27]. Therefore, sequence variety would perform the important role in conductivity properties of DNA. The results based on a DNA transistor in absent of a thermal bath show that a DNA chain with the high CG content percent behaves as a good conductor. Via the decreasing the CG content and then increasing the AT content of chain, the DNA channel shows a critical behavior. It enters to a localization-delocalization state. Via the more increasing the AT content, DNA behaves as an insulator chain. Therefore, one can choose an appropriate sequence for creating a DNA transistor. We have studied P(s) for different sequences in the contact of a thermal bath (Fig. 4-5). The bath parameter is more important than the sequence type. Here, by setting the bath parameter for all sequences, DNA channel show delocalized behavior. We can say that in the presence of a thermal bath, the effect of bath is more prominent than the effect of DNA sequence. It is clear that all of sequences show a critical behavior. None of them, even with the low CG content percent, behaves as a complete insulator. This result can show the importance of a thermal bath in molecular transistors. All P(s) diagrams are in localization-delocalization state and therefore, we can say that all of them are appropriate for designing a molecular transistor.

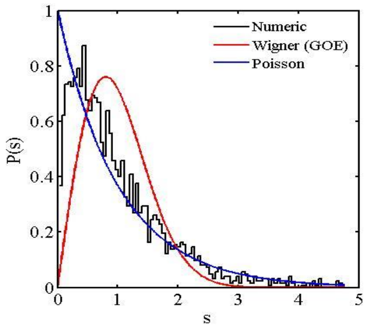

Fig. 4. Nearest neighbor level distribution for the sequence with 47% CG content.

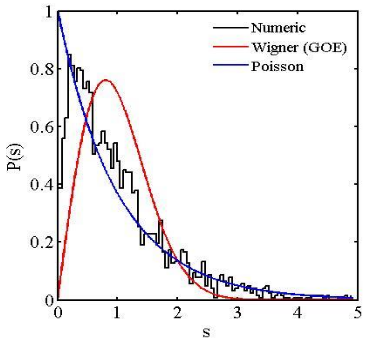

Fig. 5. Nearest neighbour level distribution for the sequence with 90% CG content.

Conclusions

We have studied the transport properties of a molecular transistor based on the DNA chain. Our aim is to determine the most appropriate setup for Designing DNA transistor. We can engineering a DNA based molecular transistor. We can show that molecular transistors can be modulated by adjustment of the bath parameters. Here, we show that by increasing the $J_{\circ} / \omega_c$ parameter of bath, one can approach to a conductivity channel. This result has been verified through the P(s) diagrams. On the other hand, we have studied the effect of DNA sequence on transport properties of transistor. It is interesting that all sequences with different CG contents, behave as an appropriate channel via the setting of bath parameters. P(s) diagrams for all sequences are in crucial state. The results based on P(s) method, show quasi-conductor channels of DNA. This results specifies the major impact of thermal bath. It can say that more effective parameter in engineering a DNA transistor is bath parameters which through the adjustment of it, we can create the most efficient molecular transistor with every DNA sequence.

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