DNA Nanowires: A Charge Transfer Approach

S. Behnia, S. Fathizadeh

Abstract—Conductivity properties of DNA molecule is investigated in a simple, but chemically specific approach that is intimately related to the Su-Schrieffer-Heeger (SSH) model. This model is a tight-binding linear nanoscale chain. We have tried to study the electrical current flowing in DNA and investigated the characteristic I-V diagram. As a result, It is shown that there are the (quasi-) ohmic areas in I-V diagram. On the other hand, the regions with a negative differential resistance (NDR) are detectable in diagram.

Keywords—Charge transfer in DNA, Chaos theory, Molecular electronics, Negative Differential resistance.

I. INTRODUCTION

IN the recent decades, DNA has increasingly interested in the potential technological applications that not directly related to the coding for functional proteins that is the expressed in form of genetic information. One of the most interesting applications of DNA is related to the construction of nanostructures of high complexity, design of functional nanostructures in nanoelectronical devices, nanosensors and nanocercuits [1]-[3]. In this field, DNA is of fundamental interest to the development of DNA-based molecular technologies, as it possesses ideal structural and molecular recognition properties for use in self-assembling nanodevices with a definite molecular architecture. Also, the robust, one-dimensional flexible structure of DNA can be used to design electronic devices, serving as a wire, transistor switch, or rectifier depending on its electronic properties. In order to understand the mechanism of the charge transport along DNA sequences, numerous studies have been carried out [4]-[6]. In this regard, conductivity properties of DNA molecule could be investigated in a simple, but chemically specific approach that is intimately related to the Su-Schrieffer-Heeger (SSH) model [7]. In SSH model, the non-diagonal matrix elements dependence on inter-site displacements is considered. In this approach, the coupling between the charge and lattice deformation is along the helix. This model is a tight-binding linear nanoscale chain established to describe conductivity phenomena in doped polyethylene. It is based on the assumption of a classical harmonic interaction between sites, which is linearly coupled to a tight-binding Hamiltonian. In this work, the Hamiltonian and corresponding motion equations are nonlinear and have high sensitivity to initial conditions. Then, we have tried to move toward the nonlinear dynamics and phase space analysis [8]. Nonlinear dynamics and chaos theory, regardless of any approximation, could open new horizons to understand the conductivity mechanism in DNA. For a detailed study, we have tried to study the current flowing in DNA and investigated the characteristic I-V diagram. As a result, It is shown that there are the (quasi-) ohmic areas in I-V diagram. On the other hand, the regions with a negative differential resistance (NDR) are detectable in diagram.

II. ANALYSIS OF THE MODEL

We have considered DNA charge transfer model via a single, simple, flexible and chemically specific model Hamiltonian. As the isolated bases in DNA are planar and the inter-base tight-binding matrix elements are small, the separation approximately holds and theories of the chemical bond appropriate to systems can be applied. In the field of conductivity phenomena in systems, the SSH model has shown a remarkable track of success for conducting polymers such as polyacetylene. Then, the DNA Hamiltonian in the presence of external field has the following form:

$$H = H_{SSH} + H_{ph} + H_{e-ph} + H_{field}. \tag{1}$$

The SSH model is used to simulate the electronic and lattice parts of system as following [9]:

$$
\begin{aligned}
H_{SSH} = &\sum_n \frac{1}{2} m \dot{x}_n^2 + \sum_n \frac{k_s}{2}(x_{n+1} - x_n)^2 \\
&+ \sum_n \varepsilon_0 c_n^+ c_n - \sum_n [t_0 - \alpha(x_{n+1} - x_n)][c_{n+1}^+ c_n + c_n^+ c_{n+1}].
\end{aligned}
\tag{2}
$$

where m is the base pair mass and x_n is the position of n-th base-pair. The energy ε_0 represents the onsite energy, c_n^+ and c_n are creation and annihilation operators of an electron. t_0 denotes the hopping integral, α is the electron-lattice coupling constant and k_s is the harmonic potential constant. The next two terms in Hamiltonian represent the vibrational mode of external phonon bath at frequency ω_0 and the local external $e-ph$ interaction term, respectively.

$$H_{ph} + H_{e-ph} = \omega_0 \sum_n b_n^+ b_n + \gamma_0 \sum_n c_n^+ c_n (b_n^+ + b_n). \tag{3}$$

where b_n^+ and b_n are creation and annihilation operators of an phonon at the site n and γ_0 is the $e-ph$ coupling constant. The external electrical field along DNA is characterized from

$$H_{field} = eE \sum_n n d c_n^+ c_n. \tag{4}$$

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where E is the uniform electrical field along the DNA chain and d is the distance between the neighboring base pairs from their equilibrium state.

In order to study the dynamics of system, we have obtained the coupled nonlinear motion equations of system based on this model. Then, we have

$$m\ddot{x}_n = k_s(x_{n+1} - 2x_n + x_{n-1})$$
$$-\alpha(c_n^+ c_{n-1} + c_{n-1}^+ c_n - c_{n+1}^+ c_n - c_n^+ c_{n+1}). \quad (5)$$

and using the Heisenberg approach

$$\dot{c}_n = -\frac{i}{\hbar}\{\gamma c_n(b_n^+ + b_n)$$
$$-[t_0 - \alpha(x_{n+1} - x_n)c_{n+1}] - [t_0 - \alpha(x_n - x_{n-1})]c_{n-1} \quad (6)$$
$$- endEc_n\}.$$

$$\dot{b}_n = -\frac{i}{\hbar}(\omega_0 b_n + \gamma_0 c_n^+ c_n). \quad (7)$$

For stability analysis, one may transform the equations into the first-order differential equations and then discrete them over time by finite difference method.

One of the key tools of nonlinear dynamics and chaos theory is Lyapunov exponent. The Lyapunov exponent is the rate at which information is lost when a map is iterated [10]. A positive value of Lyapunov exponent signifies the instable system while a negative value determines a stable one. If this quantity is computed for a sample of starting points and then averaged those results, it will be defined as the Mean Lyapunov exponent (MLE) for the system [11]. In order to investigate the characteristics of Lyapunov exponents, we introduce the $4N \times 4N$ Jacobian matrix:

$$B_{k,N} = \begin{pmatrix} X_X & X_U & X_C & X_B \\ U_X & U_U & U_C & U_B \\ C_X & C_U & C_C & C_B \\ B_X & B_U & B_C & B_B \end{pmatrix}. \quad (8)$$

The full matrix $B_{k,N}$ may be considered as a 4×4 matrix each element of which is itself a block X_X, X_U, ... that they are the derivatives with respect to the elements. Accordingly, the Lyapunov exponent is defined as [11]

$$\lambda_k = \frac{1}{4N}\ln|B_{k,N}|. \quad (9)$$

where $|B_{k,N}|$ means the determinant of matrix $B_{k,N}$.

III. RESULTS

A. Mean Lyapunov Exponent

In all of the calculations, we have used the homopolymer chain of DNA. The parameters values used in the calculation given in Table. I.

TABLE I
PARAMETERS VALUES FOR SSH MODEL

Symbol	Quantity	Value
t_0	Hopping constant	0.1 eV
α	Electron-lattice coupling constant	0.2 A^{-1}
k_s	Harmonic potential constant	0.85 eV/A^2
m	Base-pair mass	300 amu
ω_0	Bath oscillations frequency	0.1 eV
γ_0	e-ph coupling	0.01 eV

Our results show the sensitivity of the MLE to the external field. As it is shown in Fig. 1, in the SSH model, the MLE take small values when E is small and approach higher values as E varies to large values. Then, it seems that there is a critical field E_c which the system becomes unstable [12]. Then, using this method we could choose the best range of parameters affected on charge transfer in DNA. In above conditions, $E \prec E_c$ are the best ranges of the electrical field intensity so the system is stable in this region.
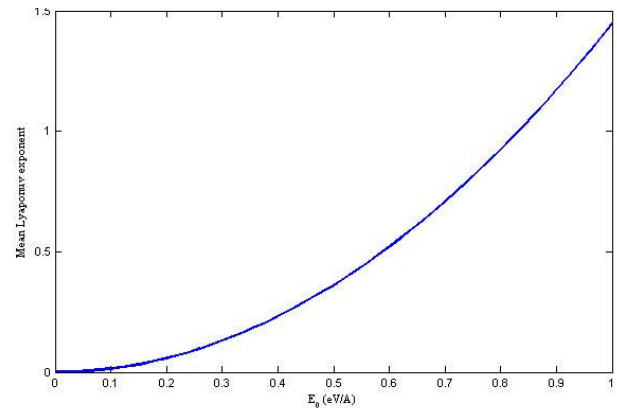

Fig. 1 Mean Lyapunov exponent with respect to the electrical field intensity

B. Electrical Current

Another factor to investigate the conductivity of DNA is the electrical current passing through it. We could calculate the time-dependent current operator as:

$$I(t) = \frac{ie}{\hbar}\sum_n [t_0 - \alpha(x_{n+1} - x_n)](c_n^+ c_{n+1} - c_{n+1}^+ c_n). \quad (10)$$

It is clear that the current is dependent on relative position of base-pairs and probability amplitude for the charge carriers in every time. As it shown, the current has the oscillatory behavior in time. At first, the current is almost regular and it has a nearly constant period but it becomes irregular over the time and oscillates with an indefinite period of time (see Fig. 2).

A. Current-Voltage Characteristic

Measurements of electrical current as a function of the potential applied across single DNA could be indicated metallic-like behaviors and efficient conduction and conversely insulator-like behaviors [13]. DNA shows different

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behaviors with respect to the variation of applied potential. In some areas it indicates quasi-ohmic behavior while in another area represents a negative slope manner. It could be shown that ohmic (quasi-ohmic) regions (with a linear gradient) and the regions with a negative gradient are distinguishable (Fig. 3). It seems that the regions with a negative gradient correspond to the negative differential resistance (NDR). NDR has been observed for DNA in the experimentally previous studies [14]. It is of special interest since it opens the possibility to develop molecular electronic switches and memory devices [15]. Recently, NDR devices have been applied to many analog and digital circuits, including logic circuit, memory circuit, frequency multiplier and divider, voltage-controlled oscillator, flip-flop circuit, and differential comparator.
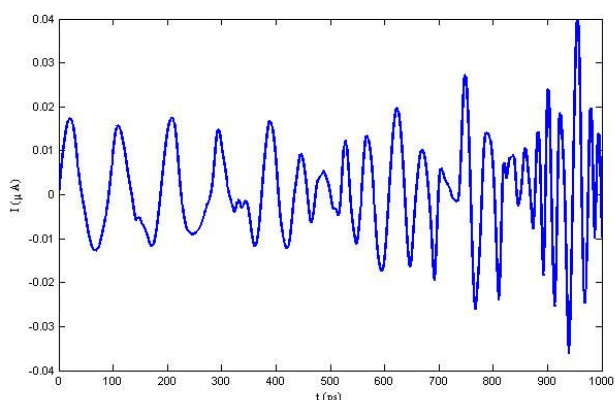

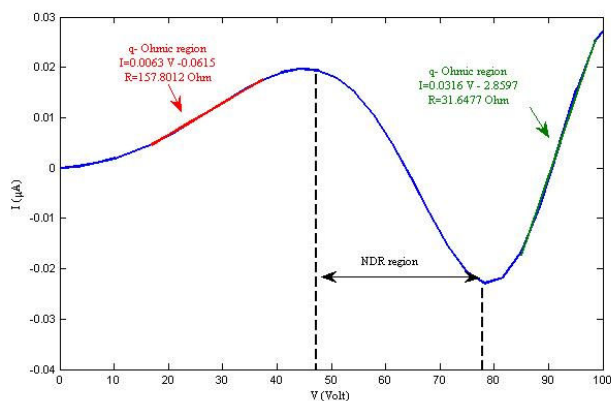Fig. 2 The electrical current time series (E=0.02 eV/A)

Fig. 3 I-V characteristic diagram in constant potential

Fig. 4 shows a three-dimensional schema of the variation of I-V characteristic in time. It is worth noting that I-V characteristic does not show any significant change in time up to 100 s which the current flowing through DNA is nearly stable. It is clear from Fig. 4 that there are the regions with quasi-ohmic or NDR properties over the time, too. However, we could apply a time periodic potential to DNA and considered I-V diagram in this situation. Fig. 5 shows the characteristic diagram in the potential $V = V_0 \cos(\omega t)$, where ω is the frequency of applied potential. We have examined the

frequency $\omega = 5$ THz for obtaining the characteristic diagram. It is clear that the quasi-Ohmic and NDR regions could also be reported. On the other hand, one could see the appearance of the neoteric quasi-Ohmic regions. The quasi-Ohmic areas change to the NDR regions and thus novel quasi-Ohmic and negative slope areas are created. Also, the width of NDR regions is reduced by increasing the voltage.
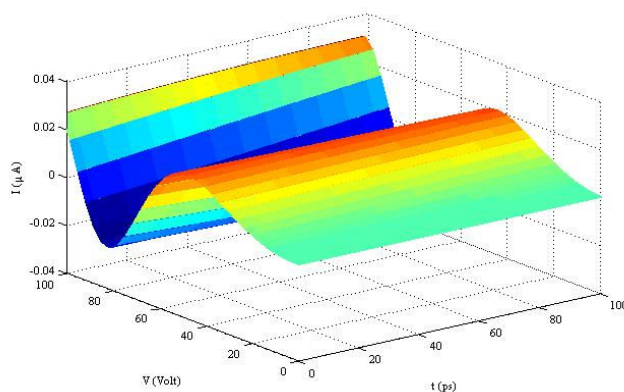

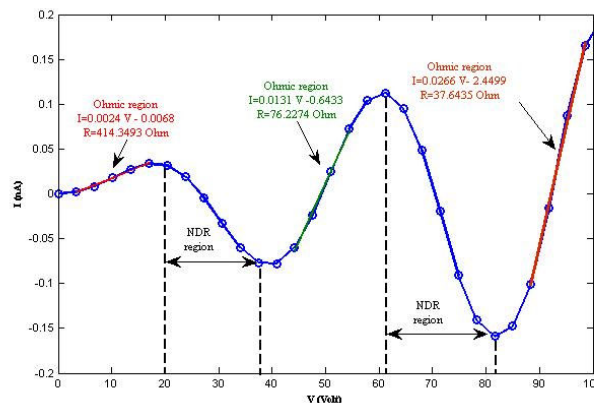Fig. 4 3-D schema of the variation of I-V in time (constant potential)

Fig. 5 I-V characteristic diagram in time periodic potential
($\omega = 5$ THz)

We could obtain the time variation of I-V characteristic diagram, too (see Fig. 6). Fig. 6 is a 3-D schema of characteristic diagram in periodic potential.

IV. CONCLUSION

We used the SSH model to investigate the interplay between the charge and lattice in DNA. It is shown that the MLE theory has helped to increase the accuracy of calculations. This makes the outcomes closer to the experimental results. The most important finding is the theoretically observation of the (quasi-) ohmic and NDR behaviors in DNA. These behaviors are revealed by the I-V characteristics at room temperature. On the other hand, by applying a time periodic potential, the novel quasi-Ohmic and NDR regions are appeared in I-V characteristic diagram. In this work, we have considered the environmental effect as a phonon bath and include its effect on the calculations.
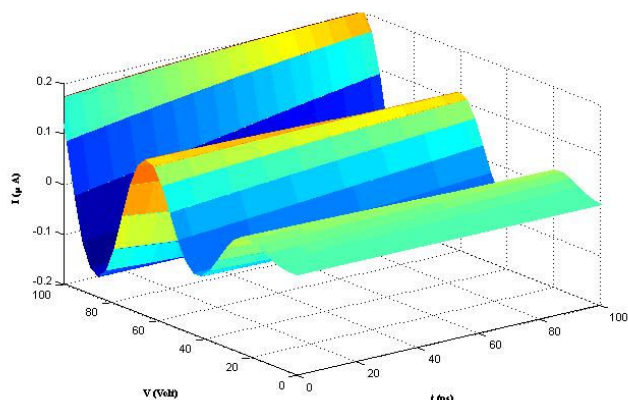
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Fig. 6 3-D schema of the variation of I-V in time (time periodic potential)

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