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 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 nanoelectronic devices, nanosensors and nanodevices [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:

\[ H = H_{SSH} + H_{ph} + H_{e-ph} + H_{field}. \]  

(1)

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

\[ H_{SSH} = \sum_{n} \frac{1}{2} m_x \dot{x}_n^2 + \sum_{n} \frac{k}{2} (x_n - x_n^0)^2 + \sum_{n} \epsilon_n c_n^+ c_n - \sum_{n} \left[ t_0 - \alpha (x_{n+1} - x_n) \right] (c_{n+1}^+ c_n + c_n^+ c_{n+1}). \]  

(2)

where \( m \) is the base pair mass and \( x_n \) is the position of \( n \)-th base-pair. The energy \( \epsilon_n \) represents the onsite energy, \( c_n^+ \) and \( c_n \) are creation and annihilation operators of an electron. \( t_0 \) denotes the hopping integral, \( \alpha \) is the electron-lattice coupling constant and \( k \) is the harmonic potential constant. The next two terms in Hamiltonian represent the vibrational mode of external phonon bath at frequency \( \omega_0 \) and the local external \( e - ph \) interaction term, respectively.

\[ H_{ph} + H_{e-ph} = \omega_0 \sum_{n} b_n^+ b_n + \gamma_0 \sum_{n} c_n^+ c_n (b_n^+ + b_n). \]  

(3)

where \( b_n^+ \) and \( b_n \) are creation and annihilation operators of an phonon at the site \( n \) and \( \gamma_0 \) is the \( e - ph \) coupling constant. The external electrical field along DNA is characterized from

\[ H_{field} = eE \sum_{n} n \epsilon_n c_n^+. \]  

(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

\[
mx''_n = k_{x}(x_{n+1} - 2x_n + x_{n-1}) - \alpha(c'_n c_{n+1} + c'_{n-1}c_n - c'_n c_{n+1} - c'_{n-1}c_n).
\]

and using the Heisenberg approach

\[
\dot{c}_n = -\frac{i}{\hbar}(c'_{n+1} + c'_{n-1}) - [t_0 - \alpha(x_{n+1} - x_{n-1})]c_{n+1} - \text{end} Ec_n.
\]

\[
\dot{b}_n = \frac{i}{\hbar}(\alpha b_n + \gamma c'_n c_n).
\]

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 unstable rate at which information is lost when a map is iterated [10].

A theory is Lyapunov exponent. The Lyapunov exponent is defined as [11]

\[
\lambda = \frac{1}{4N} \ln |B_{4N}|.
\]

where \(B_{4N}\) means the determinant of matrix \(B_{4N}\).

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>
<thead>
<tr>
<th>Symbol</th>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(t_0)</td>
<td>Hopping constant</td>
<td>0.1 eV</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>Electron-lattice coupling constant</td>
<td>0.2 Å(^{-1})</td>
</tr>
<tr>
<td>(k_x)</td>
<td>Harmonic potential constant</td>
<td>0.85 eV/Å(^{-2})</td>
</tr>
<tr>
<td>(m)</td>
<td>Base-pair mass</td>
<td>300 amu</td>
</tr>
<tr>
<td>(\omega_0)</td>
<td>Bath oscillations frequency</td>
<td>0.1 eV</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>e-ph coupling</td>
<td>0.01 eV</td>
</tr>
</tbody>
</table>

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, \(E < E_c\) are the best ranges of the electrical field intensity so the system is stable in this region.
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.

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.
Fig. 6 3-D schema of the variation of I-V in time (time periodic potential)

REFERENCES