Chaotic Modeling and Simulation (CMSIM) **1: 73-84, 2015**

Variation of Resistancec of DNA versus the Temprature

S. Behnia[1*], S. Fathizadeh[2]

[1,2] Urmia University of Technology, Orumieh, Iran
E-mail: [1] s.behnia@sci.uut.ac.ir , [2] s.fathizadeh@sci.uut.ac.ir

Abstract: In recent years DNA has attracted much attention for its potential application in molecular electronics and nanotechnology. Numerous mechanisms have been carried out for studying the charge transport in DNA. Among which a polaron hopping mechanism has turned out to be a prospective candidate for modeling the coupling between electronic and lattice configuration. In this regard, Su-Schrieffer-Heeger (SSH) model describes the coupled structural and electronics aspects of DNA. In this work Mean Lyapunov exponent (MLE) theory is proposed to study the charge transfer mechanism in DNA through SSH model. The spatial pattern of the system is disordered when MLE is large and ordered when it is small. Also, Landauer resistance is related to Lyapunov exponent via the transmission coefficient of the system. The obtained results based on the MLE theory express the effect of the temperature and external field on charge transfer and the resistance of DNA. Also it yields the best range for the field parameters.

Keywords: Charge transfer in DNA, Landaure resistance, Chaos theory, Mean Lyapunov exponent.

1. Introduction

Investigations of DNA conducting properties are very important for both classical radiobiology and quite a new science of nanobioelectronics [1]. There is clear evidence that charge injection and migration in DNA is associated with damage, mutation and repair of DNA [2]. In nanotechnology, DNA junctions have the potential of application in DNA-based drug delivery [3]. By studying the aspects of DNA single molecule conductance, it is inferred that DNA is suitable for the design of functional nanostructures in nanoelectronical devices, nanosensors, nanocercuits as well as in electrical DNA sequencing [4]. For different conditions the experimental data observed by different groups are often contradictory. Then, the argument whether DNA is a conductor [5], a

Received: 13 July 2014 / Accepted: 12 November 2014

ISSN 2241-0503

semiconductor [6] or an insulator [7] and even superconductor [8] is still ambiguous. Therefore applying the physical rules in determining the charge transfer phenomena in DNA is challenging issue. May be considering the chaos theory tools could open the new horizon in understanding the problem of charge transfer in DNA. Numerous theoretical mechanisms have been carried out for studying the charge transport in DNA. Among which a polaron hopping mechanism has turned out to be a prospective candidate for modeling the coupling between electronic and lattice configuration. The tight-binding Peyrard–Bishop–Holstein (PBH) [9,10] and Su–Schrieffer–Heeger (SSH) [11,12] are two effective models, which are all based on a polaron. In the two models, overlapping Π orbitals of the DNA base pairs are thought to provide a channel for migration of charge in it. In the current study, we have used SSH model to describe the coupled structural and electronics aspects of DNA. Also, it is important to understand how the electron transport in DNA is affected by the environmental phonons. In this model, a tight-binding nanoscale linear chain is used, which is weakly coupled to the vibrational phonon modes from the environment (reservoir) via electron– phonon (e–ph) interaction. The model, characterizes the atomic displacements as classic oscillators and charge transfer phenomena with nearest neighbor tight-binding model.

Most of the introduced Hamiltonians in DNA charge transfer and the corresponding equations of motion are extremely nonlinear and have a high sensitive behavior to chosen coefficients. Also, analysis of bioinformatics data, such as the sequences derived from the structure of DNA molecules, reveals that these data are “chaotic” in the sense that along a molecule the spatial variation is analogous to the temporal variation in chaotic systems. The Lyapunov exponent is one of the most popular concepts of the nonlinear dynamics to measure how stable the systems are. In 1999 Hiroshi Shibata introduced mean Lyapunov exponent (*MLE*) in order to characterize the chaos in systems described by partial differential equations [13, 14]. The *MLE* theory has attracted researcher’s attention and has been successfully applied in several fields [15, 16]. In this work, MLE theory is proposed to study the charge transfer mechanism in DNA through the SSH model. Also, Landaure resistance is related to Lyapunov exponent via the transmission coefficient of the system. By considering the behavior of MLE, we have studied the variation of resistance of DNA in the framework of SSH model with external phonon coupling. In the other hand, applying the electrical field, the effect of the amplitude and frequency of the field on charge transfer and resistance of DNA is studied so the best range for field parameters is selected.

2. The Model and Simulations

The studied system is consisting of the DNA lattice and an environmental optical phonon source. The Hamiltonian of the system can be modeled as

$$H = H_{SSH} + H_{Ph} + H_{e-Ph} \tag{1}$$

The first term, so-called SSH model [11, 12], has been used to simulate charge transfer in DNA with strongly internal e–ph interaction represented in classical scheme

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

where m is the mass of base pairs, t_0 is the hopping integral, the energy ε_0 is the orbital energy level of the molecule, x_n is the atomic displacement for the nth molecule, c_n and c_n^+ are creation and annihilation operators of an electron at the site n and α is the internal e–ph coupling constant. The last term in Eq. (2) represents the spring potential with an effective spring constant k_s.

Two last terms in Hamiltonian represent the vibrational mode at frequency ω_0 coming from the external sources 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 external e–ph coupling constant.

In the current study, we propose the effect of electrical field on charge transfer in DNA. In this regard, an AC field is applying so it provides an extra degree of freedom (frequency of field) in studying the effect of field. The corresponding Hamiltonian has the following form

$$H_{field} = -eE_0 \cos(\omega t) \sum_n nac_n^+ c_n \tag{4}$$

where E_0 and ω are the amplitude and the frequency of the field, respectively and $a = 3.4A^\circ$ is the distance between the base pairs in lattice.

The corresponding equations of motion have the following forms:

$$m\ddot{x}_n = k_s(x_{n+1} + x_{n-1} - 2x_n) - \alpha(c_n^+ c_{n-1} + c_{n-1}^+ c_n - c_{n+1}^+ c_n - c_n^+ c_{n+1}) + \xi_n(t)$$
$$\dot{c}_n = -\frac{i}{\hbar}\{\gamma_0 c_n (b_n^+ + b_n) - [t_0 - \alpha(x_{n+1} - x_n)]c_{n+1} - [t_0 - \alpha(x_n - x_{n-1})]c_{n-1}$$
$$-neaE_0 \cos(\omega t) c_n\}$$
$$\dot{b}_n = -\frac{i}{\hbar}(\omega_0 b_n + \gamma_0 c_n^+ c_n) \tag{5}$$

where $\xi_n(t)$ accounts for thermal noise, $\langle \xi_n(t) \rangle = 0$, $\langle \xi_n(t) \xi_k(t') \rangle = 2m\gamma k_B T \delta_{nk} \delta(t - t')$, with T as the bath temperature.

Stability analysis

The Lyapunov exponent is defined as the average rate of divergence of two initially nearby trajectories. It has been calculated for a single starting point. If we compute the Lyapunov exponent for a sample of starting points and then average those results, we define the mean Lyapunov exponent (MLE) for the system [17]. Then MLE will be a true indicator of the chaotic or nonchaotic behavior of the system. It expresses the disorderness of the spatiotemporal patterns of nonlinear systems. In order to investigate the characteristics of

Lyapunov exponents, we have used the Jacobi matrix. Jacobi matrix, gives the linear stability of the system and the disorderness of the field variables of the system. The eigenvalues of matrix give the Lyapunov exponents [13, 14]. To analyze the equations, it is convenient to transform the second order differential equations into an autonomous system of first order differential equation and use the finite difference method. Then we have

$$x_n^{i+1} = x_n^i + \Delta t u_n^i$$

$$u_n^{i+1} = u_n^i + \Delta t\{\frac{k_s}{m}(x_{n+1}^i + x_{n-1}^i - 2x_n^i) - \frac{\alpha}{m}(c_n^{i\,+} c_{n-1}^i + c_{n-1}^{i\,+} c_n^i - c_{n+1}^{i\,+} c_n^{i\,+} - c_n^{i\,+} c_{n+1}^i) + \xi_n(t)\}$$

$$c_n^{i+1} = c_n^i - \Delta t\frac{i}{\hbar}\{\gamma_0 c_n^i(b_n^{i\,+} + b_n^i) - [t_0 - \alpha(x_{n+1}^i - x_n^i)]c_{n+1}^i - [t_0 - \alpha(x_n^i - x_{n-1}^i)]c_{n-1}^i - neaE_0\cos(\omega t)c_n^i\}$$

$$b_n^{i+1} = b_n^i - \Delta t\frac{i}{\hbar}(\omega_0 b_n^i + \gamma_0 c_n^{i\,+} c_n^{i\,+}) \quad (6)$$

Then we consider the $4N \times 4N$ Jacobian matrix written as:

$$B_{k,N}=\begin{bmatrix}
\frac{\partial y_1^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial y_1^{k+1}}{\partial y_N^k} & \frac{\partial y_1^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial y_1^{k+1}}{\partial u_N^k} & \frac{\partial y_1^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial y_1^{k+1}}{\partial c_N^k} & \frac{\partial y_1^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial y_1^{k+1}}{\partial b_N^k} \\
\vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\
\frac{\partial y_N^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial y_N^{k+1}}{\partial y_N^k} & \frac{\partial y_N^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial y_N^{k+1}}{\partial u_N^k} & \frac{\partial y_N^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial y_N^{k+1}}{\partial c_N^k} & \frac{\partial y_N^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial y_N^{k+1}}{\partial b_N^k} \\
\frac{\partial u_1^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial u_1^{k+1}}{\partial y_N^k} & \frac{\partial u_1^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial u_1^{k+1}}{\partial u_N^k} & \frac{\partial u_1^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial u_1^{k+1}}{\partial c_N^k} & \frac{\partial u_1^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial u_1^{k+1}}{\partial b_N^k} \\
\vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\
\frac{\partial u_N^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial u_N^{k+1}}{\partial y_N^k} & \frac{\partial u_N^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial u_N^{k+1}}{\partial u_N^k} & \frac{\partial u_N^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial u_N^{k+1}}{\partial c_N^k} & \frac{\partial u_N^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial u_N^{k+1}}{\partial b_N^k} \\
\frac{\partial c_1^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial c_1^{k+1}}{\partial y_N^k} & \frac{\partial c_1^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial c_1^{k+1}}{\partial u_N^k} & \frac{\partial c_1^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial c_1^{k+1}}{\partial c_N^k} & \frac{\partial c_1^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial c_1^{k+1}}{\partial b_N^k} \\
\vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\
\frac{\partial c_N^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial c_N^{k+1}}{\partial y_N^k} & \frac{\partial c_N^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial c_N^{k+1}}{\partial u_N^k} & \frac{\partial c_N^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial c_N^{k+1}}{\partial c_N^k} & \frac{\partial c_N^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial c_N^{k+1}}{\partial b_N^k} \\
\frac{\partial b_1^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial b_1^{k+1}}{\partial y_N^k} & \frac{\partial b_1^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial b_1^{k+1}}{\partial u_N^k} & \frac{\partial b_1^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial b_1^{k+1}}{\partial c_N^k} & \frac{\partial b_1^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial b_1^{k+1}}{\partial b_N^k} \\
\vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots \\
\frac{\partial b_N^{k+1}}{\partial y_1^k} & \cdots & \frac{\partial b_N^{k+1}}{\partial y_N^k} & \frac{\partial b_N^{k+1}}{\partial u_1^k} & \cdots & \frac{\partial b_N^{k+1}}{\partial u_N^k} & \frac{\partial b_N^{k+1}}{\partial c_1^k} & \cdots & \frac{\partial b_N^{k+1}}{\partial c_N^k} & \frac{\partial b_N^{k+1}}{\partial b_1^k} & \cdots & \frac{\partial b_N^{k+1}}{\partial b_N^k}
\end{bmatrix} \tag{7}$$

The MLE is defined as

$$\lambda_k = \frac{1}{N}\ln\left|B_{k,N}\right| \tag{8}$$

where $\left|B_{k,N}\right|$ means the determinant of matrix $B_{k,N}$ [13,14]. A positive MLE indicates the instability of the system but its negative amount indicates the stabe system.

On the other hand, the transmission coefficient of the system (T) is given as

$$T = \exp(-2\lambda_k N) \tag{9}$$

where N is the number of base pairs in DNA lattice.

Transmission coefficient is related to the Landauer resistance via

$$\rho = \frac{1-T}{T} \tag{10}$$

in units of the quantum resistance $h/2e^2$ $(\approx 13k\Omega)$ [18].

Results and discussions

By analyzing the *MLE* theory, one could obtain the range of the parameters to have the best ordered field variables[14]. The growth of MLE corresponding to increasing the disorderness of the system then the best range for the parameters of the system is where the *MLE* takes its smaller values, which means that spatial pattern of system is ordered.

Figs. 1(a) and 1(b) show the variation of MLE and Landauer resistance with respect to the temperature in absent the external field, respectively. We have considered the case of homopolymer DNA and a length of N=100 base pairs in our numerical calculations. By considering the figures, we could see the inherently charge transfer in DNA and stability regions of the system even in absent the external current. The minimal value of the MLE and DNA resistance is about where the DNA is denatured $(\approx T = 340-350K)$.

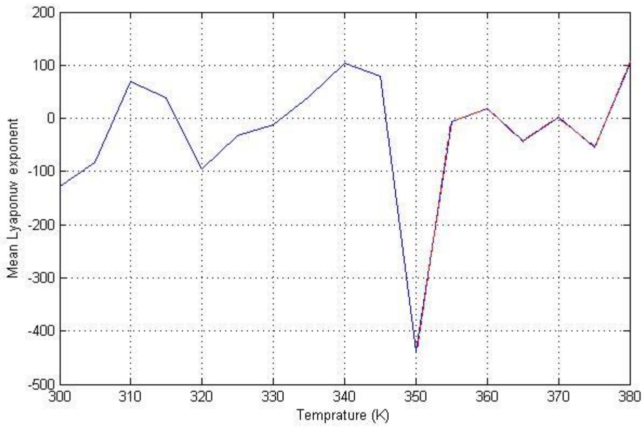

Fig. 1(a). Mean Lyapunov exponent versus the temperature in absent the external field. $t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01$.

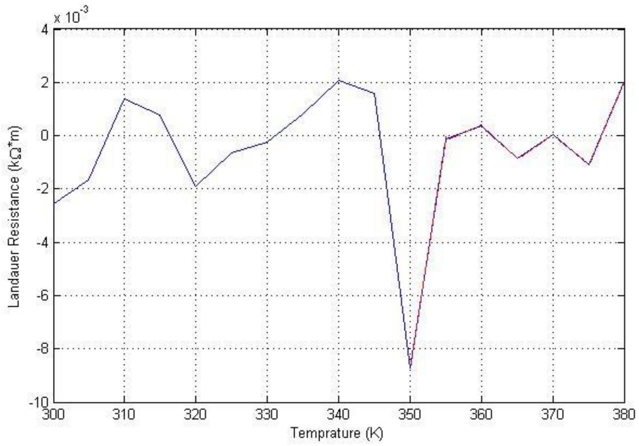

Fig. 1(b). Landauer resistance versus the temperature in absent the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01$.

Following figures appear the effect of external field with different parameters on charge transfer and resistance of DNA. We could see applying the external field decrease the resistance of DNA but the minimal value of resistance is again about where DNA is denatured.

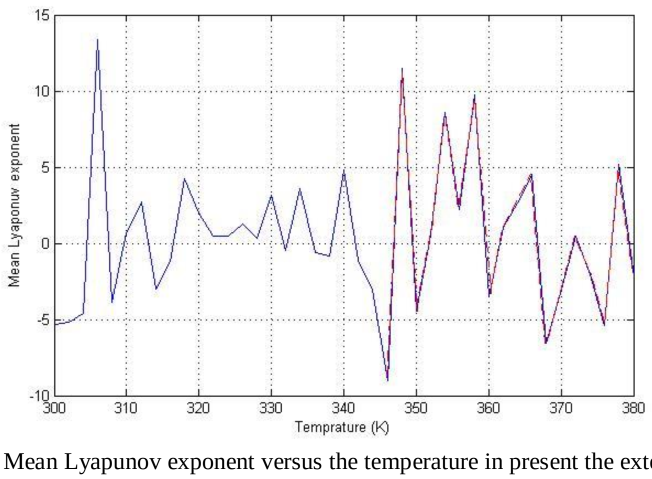

Fig. 2(a). Mean Lyapunov exponent versus the temperature in present the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, E_0 = 10, \omega = 1$.

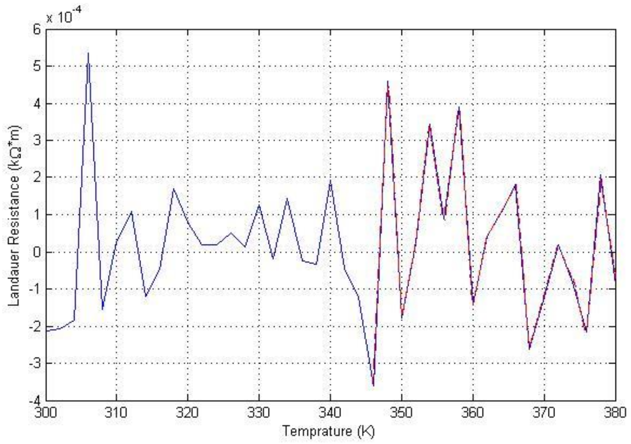

Fig. 2(b). Landauer resistance versus the temperature in absent the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, E_0 = 10, \omega = 1$.

On the other hand, by analyzing the MLE theory the best range for the parameters of the electrical field is selected, as charge current is encountered with minimal resistance.

Figs. 3 and 4 show the variations of MLE and resistance with respect to the field parameters.

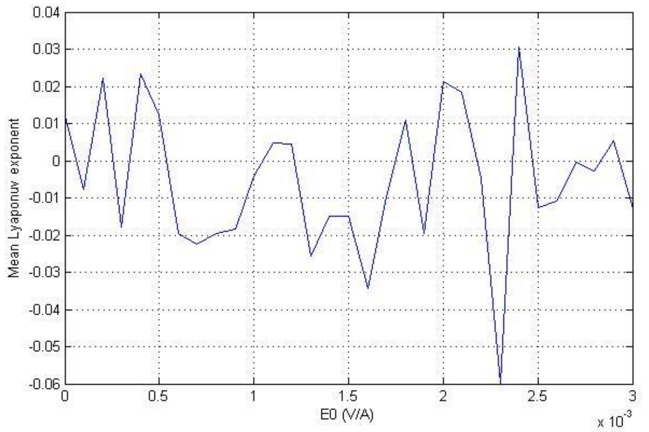

Fig. 3(a). Mean Lyapunov exponent versus the amplitude of the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, \omega = 1, temperature = 300K$.

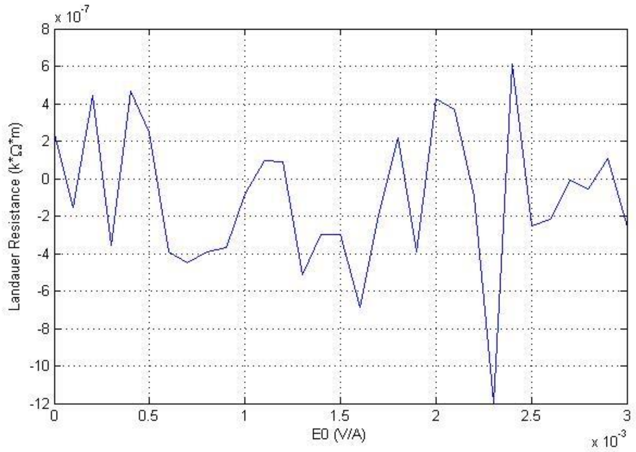

Fig. 3(b). Landauer resistance versus the amplitude of the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, \omega = 1, temperature = 300K$ ·

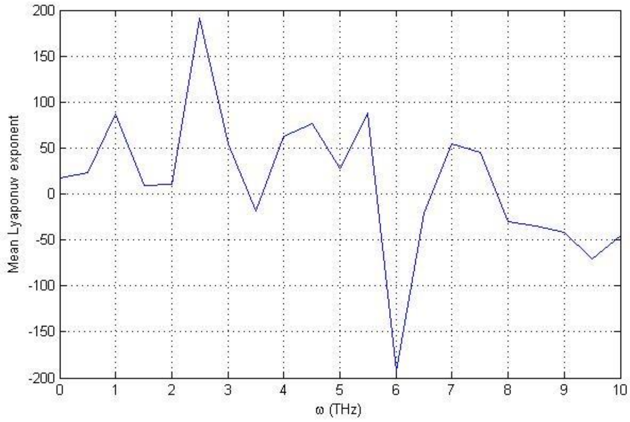

Fig. 4(a). Mean Lyapunov exponent versus the frequency of the external field.
$t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, E_0 = 2.3 mV/A, temperature = 300K$ ·

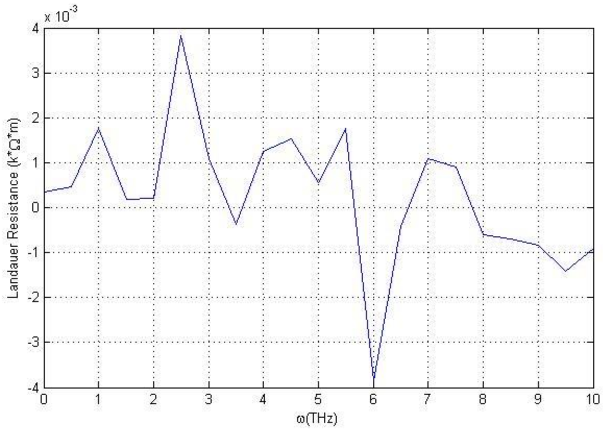

Fig. 4(b). Landauer resistance versus the frequency of the external field. $t_0 = 0.4, k = 0.85, \alpha = 0.2, \omega_0 = 0.01, \gamma_0 = 0.01, E_0 = 2.3mV/A, temperature = 300K$.

3. Conclusions

By considering the MLE, the relation between the system parameters and spatial pattern of the system is evaluated. According to the obtained results, the spatial pattern of the system is varied with respect to the parameters. In the current study, the effect of external field on charge transfer and resistance of DNA is studied. The variation of MLE and thus Landauer resistance with respect to the different parameters such as temperature, amplitude and the frequency of external field are appeared. It becomes apparent that MLE and Landauer resistance are minimal about where the DNA is denatured. On the other hand, our results show the sensitivity of *MLE* to the field parameters. Then, by considering the MLE, the best range of the system parameters is selected.

References

1. V.A. Malyshev. DNA double helices for single molecule electronics. Physical Review Letters 98: 096801, 2007.
2. S.O. Kelley and J. K. Barton. electron transfer between bases in double helical DNA. Science 283,5400: 375, 1999.
3. T. Cramer and et al. Theory and simulation of DNA charge transfer: From junctions to networks. The Journal of Physical Chemistry B 108: 16586, 2004.
4. B. M. Venkatesan and R. Bashir. Nanopore sensors for nucleic acid analysis. Nature Nanotechnology 6.10: 615, 2011.

5. H.W. Fink and C. Schönenberger. Electrical conduction through DNA molecules. Nature 398.6726: 407, 1999.
6. D. Porath and et al. Direct measurement of electrical transport through DNA molecules. Nature 403.6770: 635, 2000.
7. E. Braun and et al. DNA-templated assembly and electrode attachment of a conducting silver wire. Nature 391.6669: 775, 1998.
8. A. Yu. Kasumov and et al. Proximity-induced superconductivity in DNA. Science 291.5502: 280, 2001.
9. S. Komineas, G. Kalosakas and A. R. Bishop. Effects of intrinsic base-pair fluctuations on charge transport in DNA. Physical Review E 65.6: 061905, 2002.
10. J. Zhu and et al. Local electronic structure in the Peyrard–Bishop–Holstein model. Journal of Physics: Condensed Matter 19.13: 136203, 2007.
11. W. Su, J. R. Schrieffer and A. J. Heeger. Solitons in polyacetylene. Physical Review Letters 42.25: 1698, 1979.
12. W. Su, J. R. Schrieffer and A. J. Heeger. Soliton excitations in polyacetylene. Physical Review B 22.4: 2099, 1980.
13. H. Shibata. Lyapunov exponent of partial differential equation. Physica A: Statistical Mechanics and its Applications 264.1: 226,1999.
14. H. Shibata. Fluctuation of mean Lyapunov exponent for turbulence. Physica A: Statistical Mechanics and its Applications 292.1: 175, 2001.
15. S. Behnia and et al. A novel approach for the potential parameters selection of Peyrard–Bishop model. Physics Letters A 375.7: 1092, 2011.
16. S. Behnia and et al. Mean Lyapunov exponent approach for the helicoidal Peyrard–Bishop model. Physics Letters A 375.41: 3574, 2011.
17. R. Hilborn. Chaos and Nonlinear Dynamics, Oxford University Press, 2000.
18. L.M. Lifshits, S.A. Gredeskul, L.A. Pastur, Introduction to the Theory of Disordered Systems. Wiley, New York, 1988.