Journal of College of Education for Pure Sciences
Volume 8, Number 2, June 2018
Website: jceps.utq.edu.iq Email: jceps@eps.utq.edu.iq

Using a Nonlinear Analysis Technique, Lyapunov Coefficient, and Conductance Study on the Understanding of DNA Nanowire asa Quasi-One-Dimensional Tight-Binding Chain

Shakir A. AL-Saidi, Alaa Ayad Khedhair Al-mebir, Mohammed Hallool
Shakir.hussain@sci.utq.edu.iq , alaa_ash28@yahoo.com
Department of Physics, College of Education of Pure Sciences,
University of Thi-Qar, Nasiriyha ,Iraq

Abstract:

In this study, a nonlinear analysis technique, Lyapunov Coefficient, and the conductance measurements are used to understand the properties of DNA Nanowire as a Quasi-One-Dimensional Tight-Binding Chain. Lyapunov Coefficient for five DNA sequences including [(G/C)24], [(A/T)24], [periodic)24], [(code periodic)24] and [(random)24] were studied. Its magnitude and behavior as well as the conductance-temperature dependence are proved to be very useful for providing considerable information about DNA Nanowire system. In addition, the transmission of these five sequences and temperature-dependent conductance (vary from 0K to 300K)has been investigated.

Keywords: Lyapunov Coefficient, DNA Nanowire, Conductance, Transmission

1. Introduction

The DNA molecule, as a carrier of genetic code of all living organisms and as a promising candidate for molecular electronics, has attracted considerable attention among physics, chemistry, and biology communities recently. Since the original statement proposed by Eley and Spivey which stated that DNA could provide a natural pathway for conducting electrons[1], much progress on charge migration along duplex DNA has been achieved experimentally. The *ab initio* calculations [2-10] with form-based Hamiltonians [11-15] are generally accepted to explain the variation of experimental results and to investigate substantial electron transport mechanisms. On one hand, photoinduced experiments have demonstrated that duplex DNA could serve as a molecular bridge for long-range electron transfer on the picosecond time scale [16], or contrarily that it is somewhat more effective than protein as a mediumfor electron transfer [17]. On the other hand, the results ofdirect charge transport measurements, mainly on poly(G)-poly(C) and λ-DNA molecules, are sometimes contradict, andthey indicate that they might be insulators[18-21], semiconductors[22-24], or conductors. Such different transportstem behaviors from a wide range of experimental complications include the DNA samples, counterions, humidity,interaction of DNA with substrate, and different situations ofcontacts between DNA and electrodes.

2. Definitionofthe problem

The first case considered in this paperis the case of fishbone model that illustrated in Fig. 1. Each base pair is considered as one active region while effects of backbones are incorporated in the coupling interactions with each base site. The total number of active regions equals M. Each active region has energy sites equals to E_m with m=1,2,3,…….M.

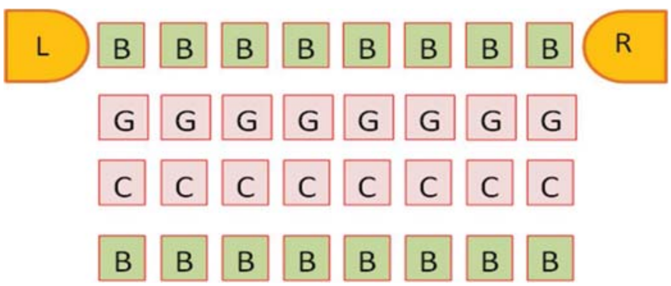

Fig.(1):A schematic illustration for the DNAas a quasi-one-dimensional model.

The model Hamiltonian that used to treat this case is given by the following time-independent one, which takes into account all sub-systems interactions,

$$\hat{H} = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_m E_m\,|m\rangle\langle m| + \sum_{k_L} E_{k_L}\,|k_L\rangle\langle k_L| + \sum_{k_R} E_{k_R}\,|k_R\rangle\langle k_R|$$
$$+ \sum_{P=\uparrow,\downarrow}\sum_{k_{bp}} E_{k_{bp}}\,|k_{bp}\rangle\langle k_{bp}| + \sum_{m=1}^{M}[V_{m,m+1}\,|m\rangle\langle m+1| + H.C.]$$
$$+ \sum_{p=\uparrow,\downarrow}\sum_{m}\left\{\sum_{k_{bp}}\left[V_{k_{bp}m}|k_{bp}\rangle\langle m| + h.c.\right]\right\}$$
$$+ \sum_{p=\uparrow,\downarrow}\sum_{k_{bp}}\left[(V_{Dk_{bp}}|D\rangle\langle k_{bp}| + H.C.) + (V_{Ak_{bp}}|A\rangle\langle k_{bp}| + H.C.)\right] + \sum_{k_L}[V_{Dk_L}|D\rangle\langle k_L|$$
$$+ H.C. + \sum_{k_R}[V_{Ak_R}|A\rangle\langle k_R| + H.C.] \ldots \qquad (1)$$

The third term is concerning to the energy sites of the active regions. $V_{m,m+1}$ represents the interaction between the nearest neighbors active regions, while $V_{k_{bp}m}$ represents the interaction between each active region with the backbone energy sites. Wave function of the system can be written as,

$$\psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_m C_m(t)|m\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle$$
$$+ \sum_{p=\uparrow,\downarrow}\sum_{k_{bp}} C_{k_{bp}}(t)|k_{bp}\rangle \ldots \qquad (2)$$

The index k_j is the energy wave vector, and the equation of motion for $C_j(t)$ can be obtained by using Schrodinger equation(in atomic unit)[19]

$$\frac{\partial\psi(t)}{\partial t} = -i\hat{H}\psi(t) \ldots \qquad (3)$$

The equations of motion for $C_j(t)$ can be obtained by using time dependent Schrodinger equation, With B_{bp} is given by[20]:

$$B_{bp}(E) = \sum_{k_{bp}}\left|V_{k_{bp}}\right|^2 \bar{\bar{C}}_{bp} = \Gamma_{bp}(E)\left\{V^{bpD}\bar{C}_D(E) + V^{bpA}\bar{C}_A(E) + \sum_m V^{bpm}\bar{C}_m(E)\right\}\ldots \qquad (4)$$

Now we define,

$$\left.\begin{aligned} d_{bpm}(E) &= \Gamma_{bp}(E)V^{bpm} \\ e_{bpm}(E) &= \Gamma_m(E)V^{mbp} \\ f_{mn}(E) &= \Gamma_m(E)V_{mn} \end{aligned}\right\}\ldots(5)$$

$\Gamma_l(E)$ is defined by eq.(15) with l=bp and m.

$$Q_{bp}(E) = \Gamma_{bp}(E)\{V^{bpD}\bar{C}_D(E) + V^{bpA}\bar{C}_A(E)\} \ldots \qquad (6)$$

Then, equations (4) and (5) are rewritten as follows,

$$B_{bp}(E) - \sum_n f_{bpm}(E)\bar{C}_m(E) = Q_{bp}(E) \ldots \qquad (7)$$

$$e_{bpm}(E)B_{bp}(E) - \bar{C}_m(E) + \sum_{m\neq n} f_{mn}(E)\bar{C}_n(E) = 0 \ \ldots \qquad (8)$$

Possibilities of connections: For the connection of both donor and acceptor with the up backbone, we can write the following,

$$\bar{C}_A(E) = \frac{V^{Ab\uparrow}B_{b\uparrow}(E)}{E - E_A - \sum_{AR}(E)}\bar{C}_D(E) \ldots \qquad (9)$$

In order to solve the system of over-mentioned related equations, the following matrix-form equation has been constructed:

$$\begin{vmatrix} -1 & d_2 & d_3 & d_4 & \bullet\bullet\bullet & d_{n-1} & d_n \\ e_{b\uparrow 1} & -1 & f_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 2} & f_{21} & -1 & f_{23} & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 3} & 0 & f_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ e_{b\uparrow m-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & f_{m-2,m-1} \\ e_{b\uparrow m} & 0 & 0 & 0 & \bullet\bullet\bullet & f_{m-1,m-2} & -1 \end{vmatrix} \begin{Vmatrix} B_{b_\uparrow} \\ \bar{C}_1 \\ \bar{C}_2 \\ \bar{C}_3 \\ \bullet \\ \bullet \\ \bar{C}_{m-2} \\ \bar{C}_{m-1} \end{Vmatrix} = \begin{vmatrix} -Q_{b\uparrow} \\ 0 \\ 0 \\ 0 \\ \bullet \\ \bullet \\ 0 \\ 0 \end{vmatrix} \qquad (10)$$

Then, by defining,

$$\Delta_\uparrow = \begin{vmatrix} -1 & d_2 & d_3 & d_4 & \bullet\bullet\bullet & d_{m-1} & d_m \\ e_{b\uparrow 1} & -1 & f_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 2} & f_{21} & -1 & f_{23} & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 3} & 0 & f_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ e_{b\uparrow m-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & f_{m-2,m-1} \\ e_{b\uparrow m} & 0 & 0 & 0 & \bullet\bullet\bullet & f_{m-1,m-2} & -1 \end{vmatrix} \qquad (11)$$

and,

$$D_{b\uparrow} = \begin{vmatrix} -1 & d_2 & d_3 & d_4 & \bullet\bullet\bullet & d_{m-1} & d_m \\ e_{b\uparrow 1} & -1 & f_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 2} & f_{21} & -1 & f_{23} & \bullet\bullet\bullet & 0 & 0 \\ e_{b\uparrow 3} & 0 & f_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ e_{b\uparrow m-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & f_{m-2,m-1} \\ e_{b\uparrow m} & 0 & 0 & 0 & \bullet\bullet\bullet & f_{m-1,m-2} & -1 \end{vmatrix} \quad (12)$$

Notably, each element in equations (10) to (12) is a function of energy, butit has been hidden for simplicity. Equation (9) can be written in the following form:

$$\bar{C}_A(E) = \frac{V^{Ab\uparrow} D_{b\uparrow 01}(E)}{(E - E_A - \Sigma_{AR}(E))D(E) - V^{Ab\uparrow} D_{b\uparrow 10}(E)} \bar{C}_D(E) \ldots \quad (13)$$

Where: $\Sigma_{kl}(E) = \left|V^{kl}\right|^2 \Gamma_l(E) \ldots (14)$

represents the interaction self-energy with:

$$\Gamma_l(E) = \sum_{k_l} \frac{\left|v_{kl}\right|^2}{E - E_{k_l}} \ldots (15)$$

With k_l=k_L , k_R , k_{Br} and k_b .

The transmission amplitude and the transmission probability [8] are respectively defined by:

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)} \ldots \quad (16)$$

and

$$T(E) = |t(E)|^2 \ldots \quad (17)$$

The Lyapunov coefficient is given by [23],

$$\gamma_N = \frac{-ln[T(E)]}{2N} \ldots \quad (18)$$

The conductance for the sequence (G/C) will be calculated as a function of temperature, *i.e.* the lead temperature, in the case of thermal equilibrium. Results will summarize for the conductance, as long as the transmission probability is obtainable in our model by using the following formula [24]:

$$G = \frac{2e^2}{h} \int_{-\infty}^{\infty} dE\, T(E) \frac{\partial f(E)}{\partial E} \ldots \quad (19)$$

$f_\alpha(E)$ is Fermi distribution function of electrons in the lead α, with α=*L, R,*

$$f_\alpha(E) = \left\{1 + \exp\left[\frac{E - \mu_\alpha}{K_B T_\alpha}\right]\right\}^{-1} \ldots \quad (20)$$

$\mu_\alpha$is the chemical potential of the lead α, with $\mu_L = \frac{V}{2}$ and $\mu_R = -\frac{V}{2}$, where V is the bias voltage. The thermal equilibrium is considered in our calculation T_R=T_L=T with $0 \leq T \leq 300\,K$.

3. Results and discussion

A fishbone model with disoriented base-pairs due to the thermal fluctuations can be viewed as a quasi-one-dimensional disordered system. In this system, the disorder leads to electronic localization. Hence, the thermal structural fluctuations will considerably limit electron transport through DNA and make electron wave functions more localized. Figures (2-4) show two plots of the transmission coefficient as a function of electron energy due to the existence of intra-coupling along the backbones, the inclusion of the hydrogen bonds between the base pairs, and the coupling between bases and backbone sites. Additionally, it can be observedthat the spectrum of transmission in (G/C) sequence is wider than (A/T) sequence due to difference between them in the energy onsite and the interactions among their components. The magnitude of the envelopes in the transmission spectrum, which initially have unit transmission, becomes suppressed and smears out below unity due to the decreasing in the number of transmitting states, while the resonance positions are shifted due to the phase changes of electrons.

Figures(2) to (7) show the energy-dependent transmission coefficient as well as the Lyapunov coefficient. They indicate transmission coefficient and Lyapunov coefficient for (a) the homogeneous poly (G/C)24 bases sequence, (b) the homogeneous poly (A/T)24 bases sequence,(c) the periodic (GA)24 sequence, (d) the periodic (AGTC)24 sequence, and (e) the random sequence, respectively.

The Lyapunov coefficient is calculated using the transmission coefficients in order to compare the transmission properties depending on the different sequences. The Lyapunov coefficient is inversely related to the localization length. If the system becomes randomized, the Lyapunov coefficient becomes bigger because the transmission has poor behavior according to the relationship, $T \propto \exp[-2\gamma L]$, where L is total length of the system. In our case, it is fixed at 24 bases.

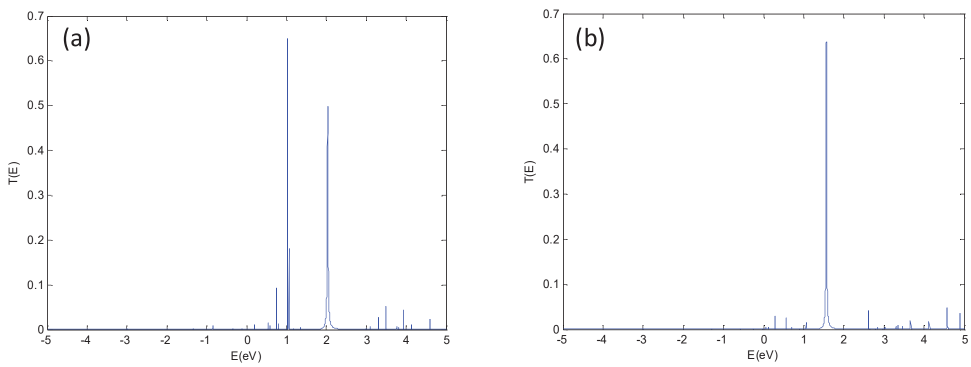

Fig.(2): Transmission probability as a function of energy at (300K) temperature and sequence: a)(G/C)24, b)(*A/T*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with

Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

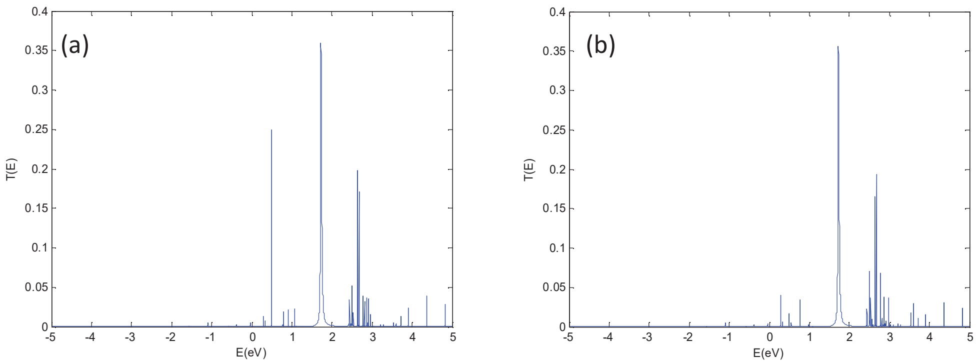

Fig.(3): Transmission probability as a function of energy at (300K) temperature and sequence: a)(periodic)24, b)(periodic code)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

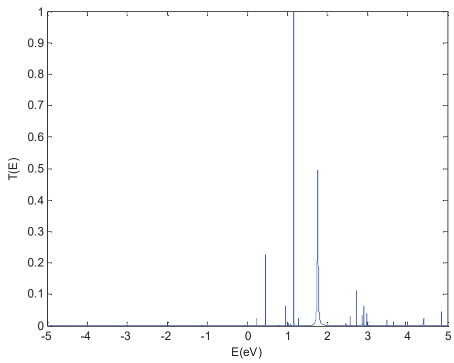

Fig.(4): Transmission probability as a function of energy at (300K) temperature and sequence (random)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

The resulting Lyapunov coefficientsare shown in Figures (5) to (7). They are zero for the protracted states in the two bands, but finite outside, showing the rapidincrease of Lyapunov coefficient out the bands. Interestingly, the behavior obtained for the sequences is in good agreement with previous theoretical studies [25], suggesting that the underlying structure of $\gamma_N(E)$given by Eq. (18) can also reflect the self-similarity associated with the partitioning of the spectrum. From an analysis over many substitutional sequences with well-organized concatenation rules, it is found that they perfectly exhibit the self-similarity. In this system, the disorder leads to electronic localization. Lyapunov coefficient reflects the level of backscattering events in the charge transport through the DNA chain. Notice that the magnitude of Lyapunov coefficient for GGGGGGGGGGGGGGGGGGGGGGGG, (AAAAAAAAAAAAAAAAAAAAAAAA)24, periodic GAGAGAGAGAGAGAGAGAGAGAGA, periodic AGTCAGTCAGTCAGTCAGTCAGTC and AAGGAAAAGAAGGGAGAAAAGAGG sequences areapproximately the same, and there are slightly wave behavior differences.The littleness of the volume of the system makes the resonance peaks more complex and, that is perhaps, by the dynamical influences which are omitted in our work.

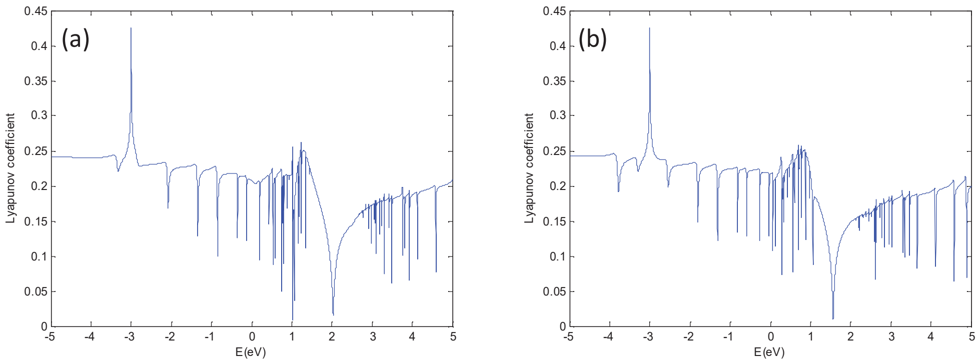

Fig.(5): Lyapunov coefficient as a function of energy at (300K) temperature with sequence: a)(G/C)24, b)(*A/T*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

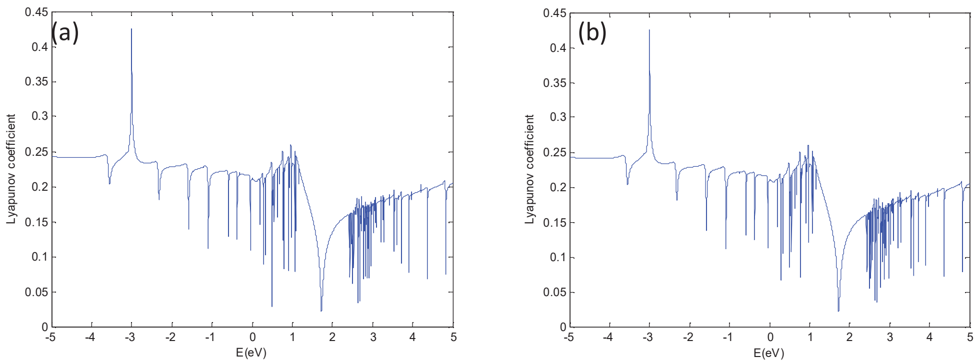

Fig.(6): Lyapunov coefficient as a function of energy at (300K) temperature with sequence: a)(periodic)24, b)(*periodic code*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

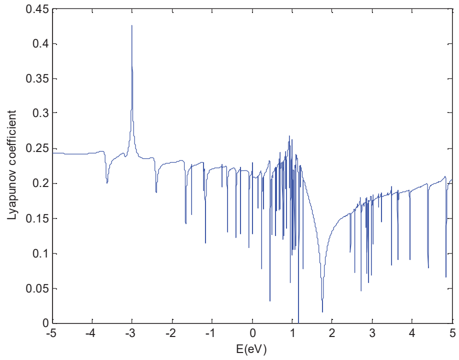

Fig.(7): Lyapunov coefficient as a function of energy at (300K)temperature with sequence (*random*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

From our results showed in Figures (8) to (10), wecan observe that the conductance is independent on temperature for 0 < T <200 K. We note that the conductance remainchangeless with the growth of temperature even it touches200 K. Whilst it is nonlinear for T >200 K at which we can observe strongincreasing suddenly in the conductance with regular increasing of temperature. This might be because of the thermal broadening of the Fermi function since our work does not include the effects of molecular vibrations. Also, strong conductance – temperature dependence at relatively high temperatures may be attributed to the access in the hybridization between the active region energy levels with the left and right leads levels as the temperature increases. For T >200 K, we can suppose that the conductance is boosted by the hopping transport mechanism between the chemical potentials and active region energy levels putting above the chemical potential and then between adjacent sites. The values of conductance are different with variation of types of sequences.

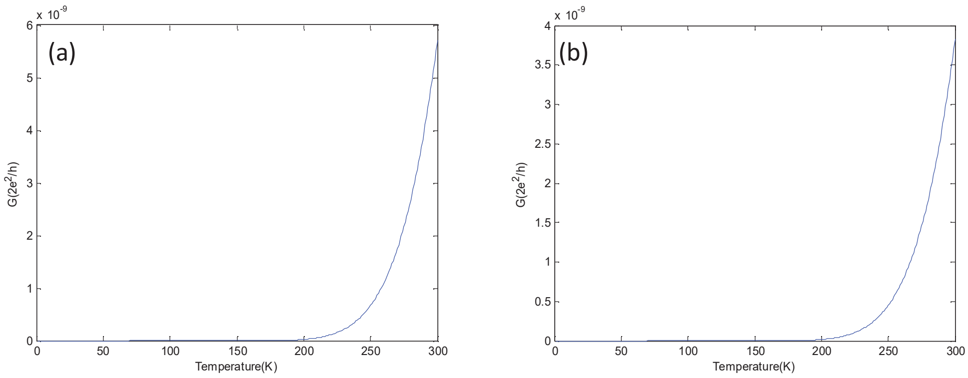

Fig.(8): Conductance as a function of temperature with sequence: a)(G/C)24, b)(*A/T*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

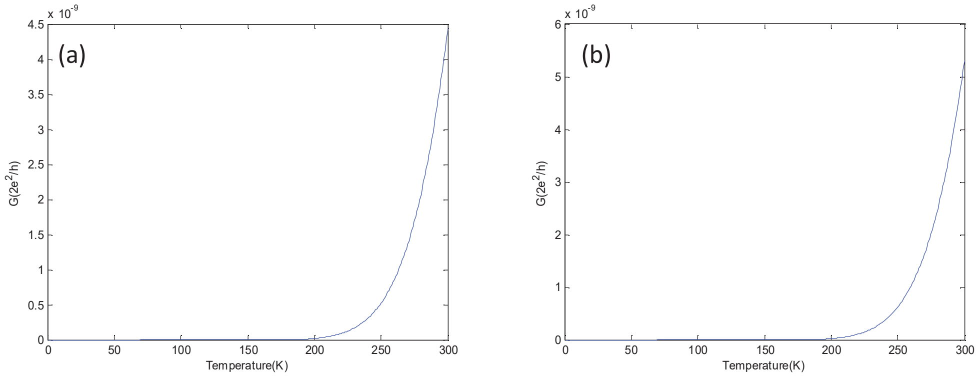

Fig.(9): Conductance as a function of temperature with sequence: a)(*period*)24, b)(periodic code) and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

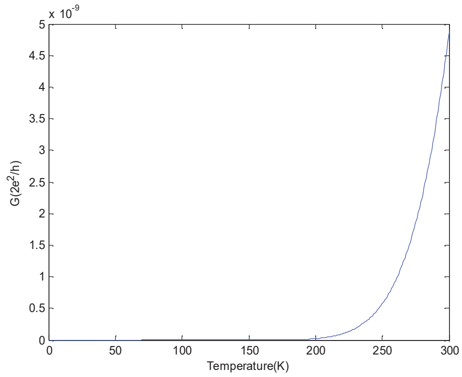

Fig.(10): Conductance as a function of temperature with sequence (*random*)24 and connections as Donor-٥-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

4. Conclusion

The results of this studycan be briefed in the following highlights. First, the degeneracy in some energy levels that make number of peak-dip transmissions is showing up less than N, also magnitudes and onsitesenergy of the transmission spectravary with kind of sequences. Second, it is noticed that the magnitude of Lyapunov coefficient for (G/C), (A/T), periodic (GA)24, periodic (AGTC)24 and (random)24 sequences are approximately the same, and since Lyapunov coefficient represents the level of backscattering events in the charge transport through the DNA chain, no clear difference was detected between sequences. Further, the conductance at $0 < T < 200$ K is approximatelyzero for all sequences, whileitisdepending on temperature at $T > 200$ K. The curves of conductance are behaving similarly for all sequences nearly, but values of conductance are varying with change of the sequences.

ACKNOWLEDGEMENTS

We thank Prof. Jenan Majeed AL-Mukh and Prof. Shakier Ibraheem Easa from Basrah University for useful discussions. We also thank Iraqi Ministry of Higher Education and Scientific Research for its support of scientific researches through the Iraqi Virtual Science Library.

Reference

[1]V. M. Kemal Bagci, Ph. D. Dissertation, University of North Texas, (2007).

[2] J. P. Lewis, P. Ordejón, and O. F. Sankey, Phys. Rev. B **55**,6880 (1997).

[3] A. A. Voityuk, J. Jortner, M. Bixon, and N. Rösch, J. Chem.Phys. **114**, 5614 (2001).

[4] Y. J. Yan and H. Y. Zhang, J. Theor. Comput. Chem. **1**, 225(2002).

[5] R. N. Barnett, C. L. Cleveland, U. Landman, E. Boone, S. Kanvah, and G. B. Schuster, J.Phys. Chem. A **107**, 3525(2003).

[6] E. B. Starikov, Philos. Mag. Lett. **83**, 699, (2003).

[7] R. Di Felice, A. Calzolari, and H. Zhang, Nanotechnology **15**,1256 (2004).

[8] H. Mehrez and M. P. Anantram, Phys. Rev. B **71**, 115405(2005).

[9] J. Ladik, A. Bende, and F. Bogar, J. Chem. Phys. **127**, 055102(2007).

[10] A. A. Voityuk, J. Chem. Phys. **128**, 115101 (2008).

[11] J. Jortner, M. Bixon, T. Langenbacher, and M. E. Michel-Beyerle, Proc. Natl. Acad. Sci. U.S.A. **95**, 12759 (1998).

[12] Y. A. Berlin, A. L. Burin, and M. A. Ratner, Chem. Phys. **275**,61 (2002).

[13] G. Cuniberti, L. Craco, D. Porath, and C. Dekker, Phys. Rev. B **65**, 241314(R) (2002).

[14] M. Unge and S. Stafström, Nano Lett. **3**, 1417 (2003).

[15] S. Roche, D. Bicout, E. Maciá, and E. Kats, Phys. Rev. Lett. **91**, 228101 (2003).

[16] Yi Jing Yan and Houyu Zhang, "Toward the mechanism of long-range charge transfer in DNA: Theories and models," Journal of Theoretical and Computational Chemistry 1 (01),225-244 (2002).

[17]Gianaurelio Cuniberti, Luis Craco, Danny Porath, and Cees Dekker, "Backbone Induced semiconducting behavior in short DNA wires," Physical review b 65 (24), 241314 (2002).

[18] Gianaurelio Cuniberti, Luis Craco, Danny Porath, and Cees Dekker, "Backbone-induced semiconducting behavior in short DNA wires," Physical review b 65 (24), 241314 (2002).

[19] D Klotsa, "RA R omer and MS Turner," Biophys J 89, 218798 (2005)

[20] D. Neuhasuer and M. Baer, J. Chem. Phys., 90, 8, 15, (1989).

[21] M. Galperin, M. A. Ratner and A.Nitzan, J. Chem. Phys. 121, 23, I (2004).

[22] T. Ihn, " Semiconductor Nanostructures: “Quantum States and ElectronicTransport",(Oxford University Press Inc.,(New York), (2009).

[23]Y. S. Joe1, S. H. Lee, E. R. Hedin, and Y. D. Kim, Journal of Nanoscience and Nanotechnology Vol. 13, 3889–3896, (2013).

[24]R. Gutierrez, S. Mandal, and G.Cuniberti, Physical Review B 71, 235116, (2005).

[25] S. LEE, MSc.Thesis, BALL STATE UNIVERSITY, (2010).