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

Modeling of electron transport in a one-dimensional tight-binding chain

S. A. A. Al-Saidi
alialimolaallp@Yahoo.com
Physics Department, College of Sciences, Thi-qar University, Iraq

Abstract
In this paper,a general formula for the transmission probability for electron transfer through the DNA system have been derived by using the steady state formalism this has been done by assuming one strand of DNA molecules as line model. TheI-V characteristics and the temperature-dependent conductance for four DNA sequences: (G-G) 24, (C-C) 24, (A-A) 24 and (T-T) 24 have been studied.

Keward; transmission, one strand,DNA

مجلة كلية التربية للعلوم الصرفة - جامعة ذي قار
المجلد ٨، العدد ٢، حزيران ٢٠١٨
Website: jceps.utq.edu.iq Email: jceps@eps.utq.edu.iq

Modeling of electron transport in a one-dimensional tight-binding chain

د. شاكر عبد الحسين السعيدي

alialimolaallp@Yahoo.com

جامعة ذي قار / كلية التربية للعلوم الصرفة /قسم الفيزياء

الخلاصة

في هذا البحث, تم اشتقاق صيغة عامة لأحتملية النفاذ لانتقال الاليكترونات خلال نظام الدنا بأستخدام صياغة الحالة المستقرة بأفتراض ان النموذج الخطي كضفيرة واحدة. مميزة التيار- فولتية واعتماد التوصيلية على درجة الحراة قد درست لأربعة انواع من سلاسل**(G-G) 24, (C-C) 24, (A-A) 24 and (T-T) 24**.الدنا:

Introduction

Charge mobility in DNA has gainedmuch attention over the recent decades, not only for its importance in biological processes [1] but also for physical applications, which use the DNA as molecular devices or by using its properties of self-assembling and self-recognition[2]. Instead of, DNA is acting as molecular wire in regularsequencesasa poly(GC), or by its doping with metalicions as is the state of M-DNA [3]. Despite the various experimental conditions and intrinsic complexities within the molecules [4–8], there isa consensus that DNA molecules, some time workingas a semiconductor with band gap is large and bandwidth is close [5,7]. An energy band shape has been adopted [9] and successfully interpret the noted current-voltage characteristics [5], and the characteristic band factors have been getting [10] for poly(G) -poly(C) and poly(A) -poly(T) via ab-initio calculations[11–14].The goal of this work is to develop a general way to get tight-binding parameters to accountinterstrand interactions from first principles. This formalism will be applied to polysG-polysC and polysA-polysTDNA.we systematically investigate the charge transfer rate in a variety of configurations of base type by usingline model.

Line Model

In the simplest single-particle tight-binding model, it has been assumed that the system can be formalized into a line model in which an effective on-site energy is used for the HOMO energy of each base. In addition to influence of the coupling between any two nearest neighbor sites. For a homogeneous DNA, such as the Poly(G), this model should be very effective due to the charge migration occuring along the purine strand in the case of the hole transport [15].We adopt the schematic model presented has been adopted in the following figure,

Fig (1) A schematic illustration of the line model. The left and right ends of the DNA(Bases)are connected to the electrode L and R in addition to D(doner) and A(accepter).

Theory and Treatment

The electron is scattered from one bridge that contains one strand of DNA. The simplest tight binding model of the DNA can be constructed as a line model. There is a single conduction channel in which sites represent bases. Every link between locationsincludes the existence of a coupling interaction. The description of DNA base as single positions represents a simplification of the line

model. This distinction becomes important when hopping between bases is considered e.g. the hopping from base to base is the same. We describe the system under consideration (that shown in Fig. (1)) by using the following time-independent Hamiltonian(using Dirac's notations).This electronic Hamiltonian takes into account all the sub-systems interactions. The different indexes D, A, L, R and b denote the donor and acceptor, the left lead, right lead, and the bridge (DNA bases with total number N). The model Hamiltonian is written as follows:

$$\hat{H} = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_{k_b} E_{k_b}|k_b\rangle\langle k_b| + \sum_{k_b}[(V_{Ak_b}|A\rangle\langle k_b| + h.c) + (V_{Dk_b}|D\rangle\langle k_b| + h.c)] + \sum_{k_R}(V_{Ak_R}|A\rangle\langle k_R| + h.c) + \sum_{k_L}(V_{Dk_L}|D\rangle\langle k_L| + h.c) \quad (1)$$

The index k_i is the energy wave vector with i types the indexes D, A, L, R and b. $E_i$types the ith energy level position and $|i\rangle$ and $\langle i|$types the ket and bra states respectively.V_{ij}types the coupling interaction between the subsystems *i* and *j*.The system wave function can be written as,

$$\psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_{k_b} C_{k_b}(t)|k_b\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle \quad (2)$$

where$C_j(t)$ types the linear expansion coefficients. The equations of motion for $C_j(t)$ can be obtained by using time dependent Schrodinger equation ,

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

So, we get the following set of related equations,

$$\dot{C}_D(t) = -iE_D C_D(t) - i\sum_{k_L} V_{Dk_L} C_{k_L}(t) - i\sum_{k_b} V_{Dk_b} C_{k_b}(t) \quad (4)$$

$$\dot{C}_A(t) = -iE_A C_A(t) - i\sum_{k_R} V_{Ak_R} C_{k_R}(t) - i\sum_{k_b} V_{Ak_b} C_{k_b}(t) \quad (5)$$

$$\dot{C}_{k_b}(t) = -iE_{k_b} C_{k_b}(t) - iV_{k_bD} C_D(t) - iV_{k_bA} C_A(t) \quad (6)$$

$\dot{C}_{k_L}(t) = -iE_{k_L}C_{k_L}(t) - iV_{k_L D}C_D(t)$(7)

$\dot{C}_{k_R}(t) = -iE_{k_R}C_{k_R}(t) - iV_{k_R A}C_A(t)$ (8)

With, $V_{ij} = V_{ji}$ and i , j=A , D , k_L , k_R and k_b

By using condition stationary states, we define $C_j(t)$ as $C_j(t) = \bar{C}_j e^{-iEt}$ with E types the system eigen values. So we put$\dot{\bar{C}}_j = 0$. Then follow separation procedure:

$V_{k_i \alpha} = v_{ki} V^{I\alpha}$ (9)

$\overline{C}_{ki} = v_{ki}\bar{\bar{C}}_I$ (10)

With *i*=L, R and b and α=A, D and b

By substituting these definitions in eqs.((4)-(8)) we get, .

$$\bar{C}_A(E) = \frac{1}{E - E_A}\left\{V^{AR}\sum_{k_R}|v_{k_R}|^2\bar{\bar{C}}_R + V^{Ab}\sum_{k_b}|v_{k_b}|^2\bar{\bar{C}}_b\right\} \quad (11)$$

$$\bar{C}_D(E) = \frac{1}{E - E_D}\left\{V^{DL}\sum_{k_L}|v_{k_L}|^2\bar{\bar{C}}_L + V^{Db}\sum_{k_b}|v_{k_b}|^2\bar{\bar{C}}_b\right\} \quad (12)$$

$$\bar{\bar{C}}_b(E) = \frac{1}{E - E_b}\{V^{bD}\bar{C}_D + V^{bA}\bar{C}_A\} \quad (13)$$

$$\bar{\bar{C}}_L(E) = \frac{1}{E - E_L}V^{LD}\bar{C}_D \quad (14)$$

$$\bar{\bar{C}}_R(E) = \frac{1}{E - E_R}V^{RA}\bar{C}_A \quad (15)$$

Thus, we obtain an obvious expression for

$$\frac{\bar{C}_A(E)}{\bar{C}_D(E)} = \frac{X_1(E)}{X_2(E)} \quad (16)$$

Where

$$X_1(E) = V^{Ab}\Gamma_b(E)V^{bD} \quad (17)$$

$$X_2(E) = E - E_A - \sum\nolimits_{AR}(E) - \sum\nolimits_{Ab}(E) \quad (18)$$

Where,

$\sum_{ij}(E) = |V^{ij}|^2\Gamma_j(E)$ (19)

is the interaction, self-energy, with,

$$\Gamma_j(E) = \sum_{k_j}\frac{|v_{k_j}|^2}{E - E_{k_j}} \quad (20)$$

With $k_j=k_L$,k_R and k_b .

The transmission amplitude and the transmission probability are respectively defined as:

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)} \qquad (21)$$

and ,

$$T(E) = |t(E)|^2 \qquad (22)$$

The results and discussion

To begin with, the eigenvalues of the bases (arranged in homogenous sequence) are calculated by using tight binding model[15],

$$E_j = E_{basis} - 2V_{nm}\cos(\frac{\pi j}{N+1}) \quad (23)$$

Where, E_{basis} is the energy of the base, which is given by E_G (=-2.63eV), E_C (=-3.75eV), E_A (=-3.25eV) and E_T (=-4.15eV) [8],forthe Guanine, Cytosine, Adenine and Thymine respectively, which are putting in the LUMO levels[15]. The coupling interaction between nearest-neighbor bases refer to it by V_{nm}, where V_{nm}=0.119 eV and -0.38 eV for both (G-G) and(C-C) and both (A-A) and (T-T) respectively. The single base is j and the total number of the bases is N. The energy levels locationsin this case are putting in the range2.64 ≤ E ≤ 3.11eV,1.52 ≤ E ≤ 1.99 eV, 2.17 ≤ E ≤ 2.32 eV and 1.27 ≤ E ≤ 1.42 eV for (G-G)24, (C-C)24, (A-A)24 and (T-T)24 sequence respectively,theyare putting in the LUMO levels. So that, the density of states is writing as,

$$\rho(E_j) = \frac{N}{2\pi}\frac{1}{|t|\sin(\frac{\pi j}{N+1})} \qquad (24)$$

The plotting of the transmission probability T (E) and energy E relationshipin the case that come back to the active region, which consist of the DNA bases only aregiven as follows:

Figs.((2)-(5)) show the results obtained, considering the line model with the sequence (G-G)24, (C-C)24, (A-A)24 and (T-T)24, using the factors V^{Ab}=- 0.9 eV and V^{bD} =-0.5 eV. Where, we note that many of the states close to the active region edges own a very low transmission probability. While high transmission probability will be at locations near energies of bases, since the coupling between them is turn on, alsothe shapes of the curves are changing with kind of sequence. This is reasonable because the coupling interactions of the active region with the donor and accepter are inequality,add to, the energy location is dependent on the sequence. Because the degeneracy in some energy levels the number of peak-dip transmissions isseemfewer than N,and emerge ofthese resonances are due to the interference of coupling interactions. The transmission spectrum(magnitude and location) is changing with thekind of sequence. Calculations of the transmission spectrum are the most important

step in studying the transport and dynamic properties of the electron mobility process in nanostructures. Our transmission spectrum calculations will be used to find the electric current through the DNA molecule. The steady state electric current through the active region can be accounted by using the Landauer formula [16]:

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_L(E) - f_R(E)]dE \qquad (25)$$

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

$$f_\alpha(E) = \left\{1 + \exp\left[\frac{E-\mu_\alpha}{K_B T_\alpha}\right]\right\}^{-1} \qquad (26)$$

$\mu_\alpha$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.While T_α is the temperature of the lead α, with T_L=T_R=T, T is fixed at 300K, this namely that both leads are in thermal equilibrium state.

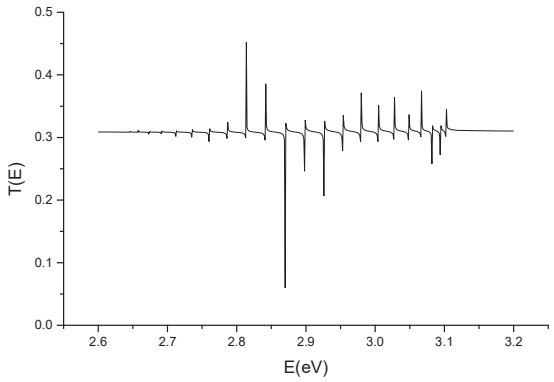

Fig. (2)Transmission as function of energy for sequence (G-G) 24.

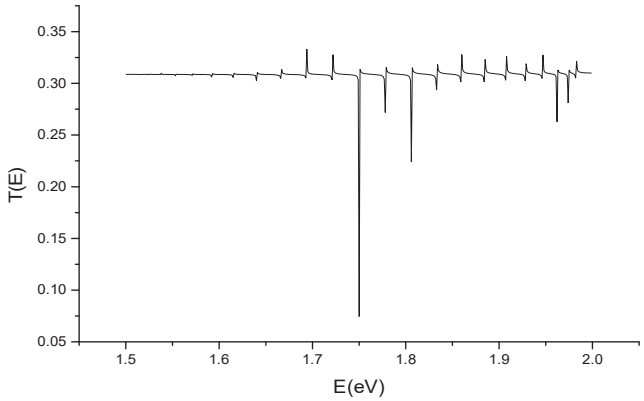

Fig. (3) Transmission as function of energy for sequence (C-C) 24.

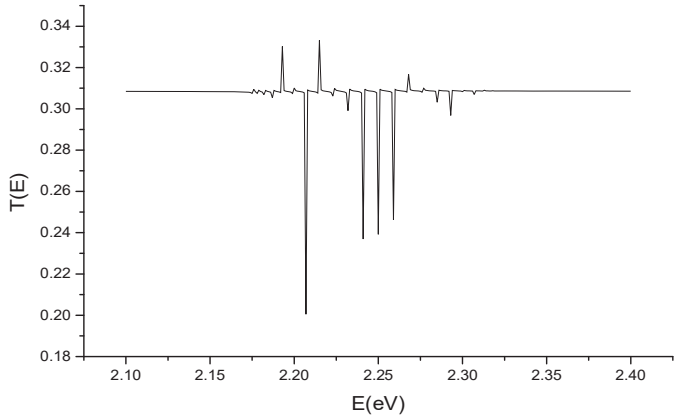

Fig.(4) Transmission as a function of energy for the sequence (A-A) 24.

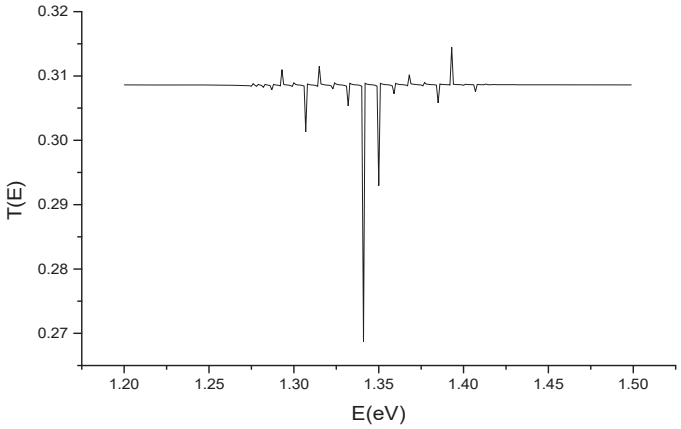

Fig. (5) Transmission as a function of energy in sequence (T-T) 24.

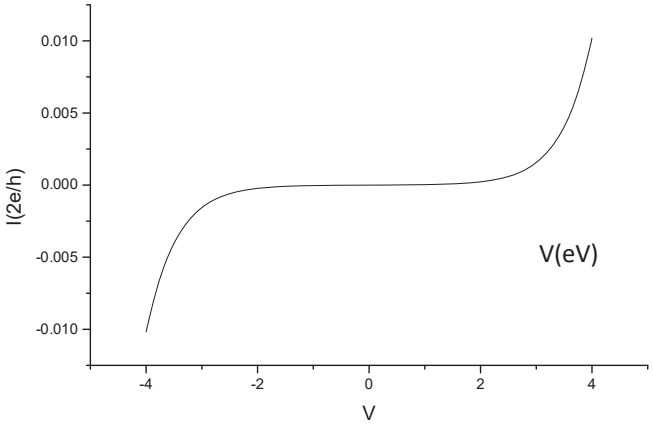

Fig.(6) Current as a function of bias voltage with sequence (G-G) 24 for line model.

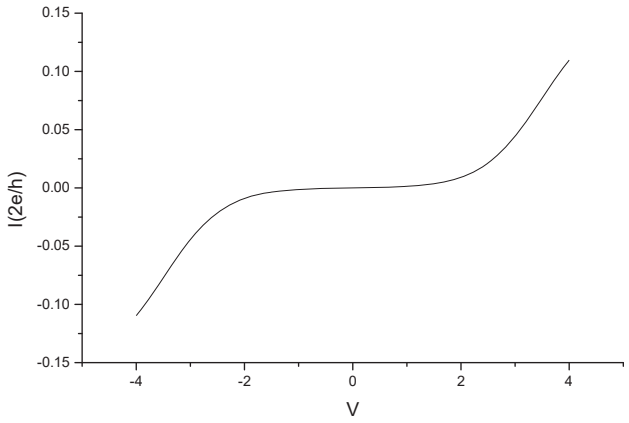

Fig (7) Current as a function of bias voltage with sequence (C-C) 24 for line model.

V(eV)

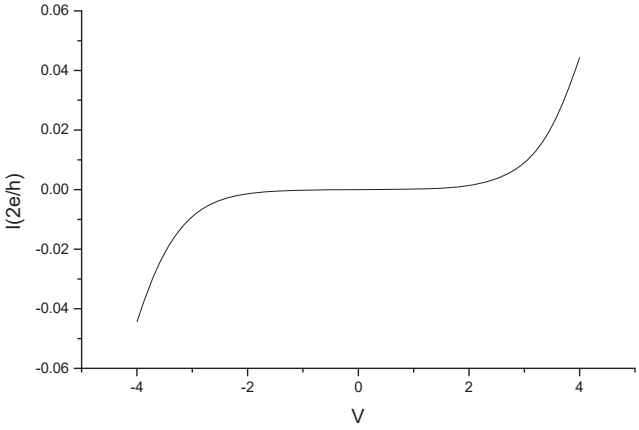

Fig.(8) Current as a function of bias voltage with sequence (A-A) 24 for line model.

V(eV)

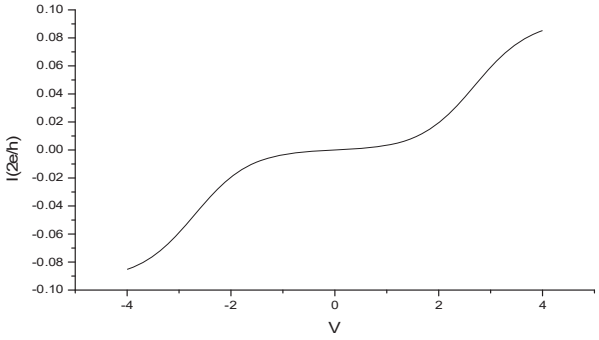

Fig (9) Current as a function of bias voltage with sequence (T-T) 24 for line model.

The tunneling current calculation V(eV)

The tunneling current properties are investigated by oscillating the bias voltage from -4 eV to 4 eV. The I-V curves for the same over mentioned connections are shown over the extended bias window as shown in the Figs.((6)-(9)). The *I-V* curves clearly show a nonlinear dependence. Overlap of electrons in single molecule is aninnovator influence and has some like overlap on dual slits. It appears itself as ideal destructive overlaps that lead tofullstopping of the current through the molecule and has been expected for molecules with separatealternating symmetry. The symmetry asserts the existence of degenerate states, to which clockwise and counter-clockwise angular momenta can be assigned, so that the two pathwaysabout the molecule display a finite phase variationrelying on the aligning of the contacts. From these figures, as the active region has steady order, we can evidentially distinguish two orders. To begin with, the current is minish for finiteextent of bias voltage. This energy gap is type- sequence-dependent.Wherewe can observe the gap of (G-G) and (A-A) is greater than the gap of (C-C) and (T-T).All figures illustrate that the DNA is operating as an alienator in low voltage bias. At bias voltages greater than the absolute value of the energy gap,the current shows avigorous increase as shown in all figures.Also observable is the actuality that the I-V characteristics are nearly symmetric with respect to the absolute value of the bias polarity, since the active region is falling in the mid gap between the electrodes therefore, this variable in the current level and conductivity perhapsexplain by the difference of resistance values. Our results giveanall right qualitative acceptance with the electronic structure(*i.e.*the transmission spectrum) of the system with the part of current near zero of the *I-V* curves. The values of energy gap may also powerfully depend on the clutter and connection which are not included in our work.

The Conductance Calculations

The conductance for the sequence (G-C) will be accounted as a function of temperature, *i.e.* the lead temperature, in the thermal equilibrium state. Our results for the conductance will summarize, as long as the transmission probability is obtainable in our model computation,by using the nextform [17]

$$G = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\, T(E)\frac{\partial f(E)}{\partial E} \quad (26)$$

With *f(E)* is defined in eq(29).As the thermal equilibrium is considered in our calculation $T_R=T_L=T$ with $0 < T < 300$ K. Our results are presented in figs.((10)-(13)) are with one strand model. The conductance is autonomic withthe temperatureat $0 < T < 200$ K, $0 < T < 150$ K, $0 < T < 175$ K and $0 < T < 130$ K, for (G-G), (C-C), (A-A) and (T-T)respectively. The conductance remains constant with eking of temperature until it becomesapproximately 200,150,175 and 130K for (G-G), (C-C), (A-A) and (T-T) respectively. While it is nonlinear at $T > 200$ K, $T > 150$ K,$T > 175$ K and $T > 130$ K for

(G-G), (C-C), (A-A) and (T-T) respectively, at these values of temperature high and ferlyeking in the conductance with regular eking of temperature. It is too fastidious to interpret the observed temperature relyingonDNA. According to our treatment,the strength of the conductance – temperaturerelying at relatively high temperatures can be returned to the eking in the hybridization between the active region energy levels with the left and right lead levels as the temperature eking. For T > 200 K, T > 150 K, T > 175 K and T > 130 K for (G-G), (C-C), (A-A) and (T-T) respectively, by the hopping transport mechanism between the chemical potentials and active region energy levels (whichputtingup the chemical potential and then between neighboring locations) the conductance is cementing. They interpret the temperature relying conductivity proposing two transport mechanisms, i.e. ionic conduction at low temperatures and temperature driven hopping transport operations at high temperatures. The foundation physics of the weak temperature relying at low temperatures is returned to the electrons in the molecules have not enough energy to participate of conductance.

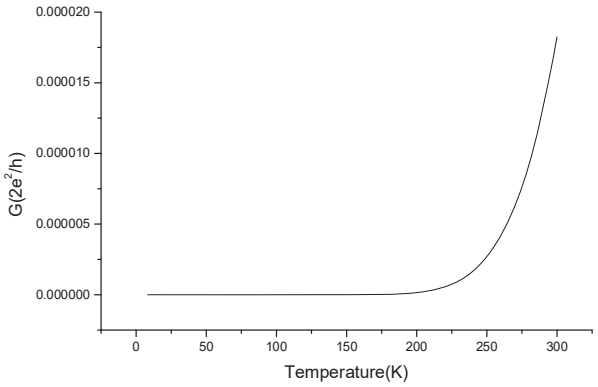

Fig.(10) Conductance as a function of temperature with sequence (G-G) 24 for line model.

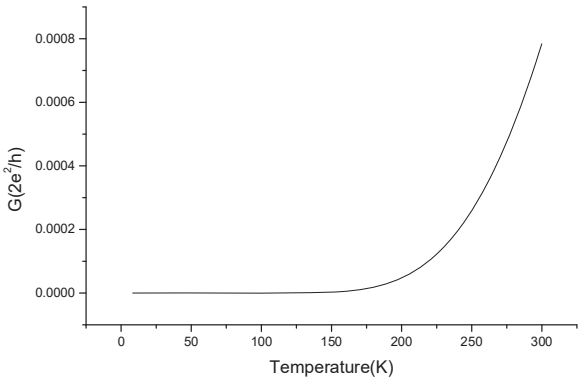

Fig.(11) Conductance as a function of temperature with sequence (C-C) 24 for line model.

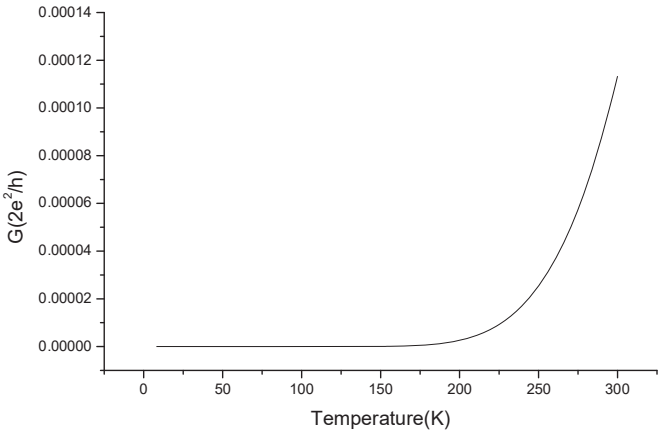

Fig.(12) Conductance as a function of temperature with sequence (A-A) 24 for line model.

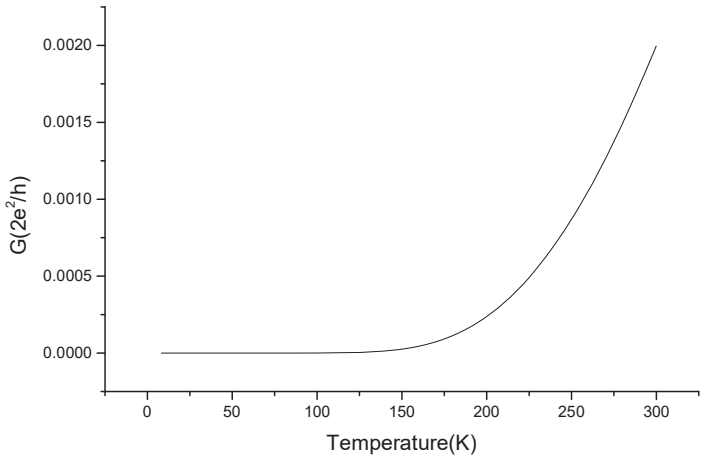

Fig.(13) Conductance as a function of temperature with sequence (T-T) 24 for line model.

Conclusion

Finally, the results can be summarized as follow:

1) The number of peak-dip transmissions is appearing less than N, because of the degeneracy in some energy levels.

The transmission spectrum (magnitude and onsite) changes with the type of sequence.

2) The *I-V* curves clearly show a nonlinear dependence. The *I-V* curves shapes are alike for four sequences, but they are not equal in the bias voltage gap(namely, values of bias voltage which have zero current).

3) The conductance is independent of temperature at $0 < T < 200$ K, $0 < T < 150$ K, $0 < T < 175$ K and $0 < T < 130$ K, for (G-G), (C-C), (A-A) and (T-T) respectively. While it is nonlinear at $T > 200$ K, $T > 150$ K, $T > 175$ K and $T > 130$ K for (G-G), (C-C), (A-A) and (T-T) respectively, at these values of temperature high and sudden increasing in the conductance with normalincreasing of temperature. The curve of conductance is behavior similarly for all sequence nearly.

ACKNOWLEDGEMENTS

We thank Prof. JenanMajeed AL-Mukh and Prof. Shakier IbraheemEasa 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.

References

[1]G. B. Schuster Ed., vol. 236/237 of Topics in Current Chemistry (Springer, Berlin, 2004).

[2]K. Keren, R. S. Berman, E. Buchstab, U. Sivan, and E. Braun, Science 302,1380 (2003); M. Mertig, R. Kirsch, W. Pompe, and H. Engelhardt, Eur. Phys. J. D 9, 45 (1999).

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

[4]A. J. Storm, J. V. Noort, S. D. Vries and C. Dekker,Appl. Phys. Lett. 79, 3881 (2001).

[5]D. Porath, A. Bezryadin, S. de Vries and C. Dekker,Nature 403, 635 (2000).

[6]H. Cohen, C. Nogues, R. Naaman and D. Porath, Proc.Natl. Acad. Sci. U.S.A. 102, 11589 (2005).

[7]K.-H. Yoo, D. H. Ha, J.-O.Lee, J. W. Park, J. Kim, J.J. Kim, H.-Y. Lee, T. Kawai and H. Y. Choi, Phys. Rev.Lett. 87, 198102 (2001).

[8]B. Xu, P. Zhang, X. Li and N. Tao, Nano Lett. 4, 1105(2004).

[9]M. Hjort and S. Stafstr¨om, Phys. Rev. Lett. 87, 228101(2001).

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

[11]S. Datta, Electronic Transport in Mesoscopic Systems(Cambridge University Press, Cambridge, 1999).

[12]S. Datta, Quantum Transport: Atom to Transistor(Cambridge University Press, Cambridge, 2005).