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Steady State Formalism for Electron Transfer through DNA System: Ladder Model

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Abstract: ***General steady state formalism for the transmission probability for electron transfer through DNA system is derived, by assuming DNA system chain as one scattering region bounded by two strands. The ladder model is considered to calculate the energy spectrum of the DNA system. The transmission probability calculations are employed to calculate I-V characteristics and the temperature-conductance dependence which are found to be comparable in behavior with other findings.***

Keywords: Nano science, DNA, ladder model, *I-V* characteristics, transmission probability

1. Introduction

In order to obtain estimates of quantum transport at the molecular scale, electronic structure calculations must be plugged into a formalism which would eventually lead to observables such as the linear conductance (equilibrium transport) or the current-voltage characteristics (non-equilibrium transport). Within the class of biopolymers, DNA is expected to play an outstanding role in molecular electronics. This is mainly due to its unique self-assembling and self-recognition properties which are essential for its performance as a genetic code carrier. It is the hope of many scientists that these properties might be further exploited in the design of electronic circuits [1-4]. Recently, experiments [5] on single suspended DNA with a more complex base sequence have shown unexpectedly high currents of the order of 100–200 nA. The theoretical interpretations of these recent experiments and, in a more general context, the elucidation of possible mechanisms for charge transport in DNA have not, however, been unequivocally successful so far. While ab initio calculations can give at least in principle a detailed account of the electronic and structural properties of DNA, the huge complexity of the molecule and the diversity of interactions present preclude a complete treatment for realistic molecule lengths. On the other hand, model-based Hamiltonian approaches to DNA have been already been discussed in great detail and can play a role by addressing single factors that influence charge transport in DNA. In order to mirror the experimental situation, a large variety of theoretical studies have been modeled but the results are not necessarily consistent across different models. In this model, each base is modeled as a distinct site where the base pair is then weakly coupled by the hydrogen bonds. The resulting two-channel model is shown in Fig.(1). This ladder model is a planar projection of the structure of the DNA with its double helix unwound. There are two central branches, linked with one another, with interconnected sites where each represents a complete base and which are additionally linked to the upper and lower backbone sites. The backbone sites as in the fishbone model are not interconnected. The hydrogen-bonding between base-pair is described as an additional hopping perpendicular to the DNA stack as shown in Fig.(1). In the following, we will present our extended theoretical treatment for both the case of the electron scattered from one scattering region that contains base pairs only and the one contains both the base pairs and the backbone to calculate transmission probability as a function of electron energy from which we obtain all the transport properties.

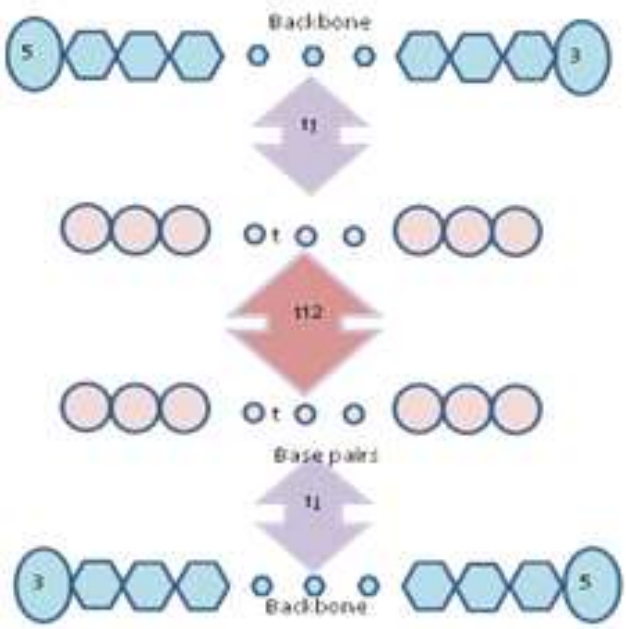


Figure 1: The ladder model for electron transport along DNA.

2. Theoretical Model

2.1 The Case of Active Region contains the base pairs only

The simplest tight binding model of the DNA stack can be constructed as a one dimensional model. There is a single central conduction channel in which the individual sites represent a base-pair. Every link between sites implies the presence of a coupling interaction. The description of DNA base pair as a single site represents a simplification of the wire model. Accordingly, the distinction will be loosed between a pair with G (or A) on the 5' end of the DNA and a C (or T) on the 3' side and one where C sits on the 5' and G

on the 3', *i.e.* GC is equal to CG. This distinction becomes important when considering hopping between base-pairs, e.g. the hopping from GC to AT is different from CG to AT because of the different size of the DNA bases and thus the different overlap between G to A and C to A (and similarly for C to T and G to T) [6]. We describe the system under consideration (that shown in fig.(1, a) 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, Br, L, R, $b_\uparrow$ and $b_\downarrow$ denote the donor and acceptor, the bridge (DNA molecules bases with total number N), the left lead and right lead, and the up and down backbones. The model Hamiltonian is as follow,

$$\begin{aligned}\hat{H} &= E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_{k_{Br}} E_{k_{Br}}|k_{Br}\rangle\langle k_{Br}| \\ &+ \sum_{k_L} E_{k_L}|k_L\rangle\langle k_L| + \sum_{k_R} E_{k_R}|k_R\rangle\langle k_R| \\ &+ \sum_{q=\uparrow,\downarrow}\sum_{k_{bq}} E_{k_{bq}}|k_{bq}\rangle\langle k_{bq}| + \sum_{q=\uparrow,\downarrow}\sum_{k_{bq}}[(V_{Ak_{bq}}|A\rangle\langle k_{bq}| + h.c) \\ &+ (V_{Dk_{bq}}|D\rangle\langle k_{bq}| + h.c) + \sum_{k_{Br}} V_{k_{Br}k_{bq}}|k_{Br}\rangle\langle k_{bq}| + h.c)] \\ &+ \sum_{k_R}(V_{Ak_R}|A\rangle\langle k_R| + h.c) + \sum_{k_L}(V_{Dk_L}|D\rangle\langle k_L| + h.c) \qquad (1)\end{aligned}$$

The index $k_i$is the energy wave vector. E_i represents the ith energy level position and $|i\rangle$ and $\langle i|$ represent the ket and bra states respectively. V_{ij} represents the coupling interaction between the subsystems i and j with $V_{ij}= V_{ji}$. The system wave function can be written as,

$$\begin{aligned}\psi(t) &= C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_{k_{Br}} C_{k_{Br}}(t)|k_{Br}\rangle + \\ &\sum_{q=\uparrow,\downarrow}\sum_{k_{bq}} C_{k_{bq}}(t)|k_{bq}\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle \quad (2)\end{aligned}$$

Where $C_j(t)$ represent the time dependent expansion coefficients. The equations of motion for $C_j(t)$ can be obtained by using time dependent Schrodinger equation [7],

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

So, we get the following set of related differential equations,

$$\dot{C}_D(t) = -iE_DC_D(t) - i\sum_{k_L} V_{Dk_L}C_{k_L}(t) - i\sum_{q=\uparrow,\downarrow}\sum_{k_{bq}} V_{Dk_{bq}}C_{k_{bq}}(t) \quad (4)$$

$$\dot{C}_A(t) = -iE_AC_A(t) - i\sum_{k_R} V_{Ak_R}C_{k_R}(t) - i\sum_{q=\uparrow,\downarrow}\sum_{k_{bq}} V_{Ak_{bq}}C_{k_{bq}}(t) \quad (5)$$

$$\begin{aligned}\dot{C}_{k_{bq}}(t) &= -iE_{k_{bq}}C_{k_{bq}}(t) - i\sum_{k_{Br}} V_{k_{bq}k_{Br}}C_{k_{Br}}(t) - \\ &iV_{k_{bq}D}C_D(t) - iV_{k_{bq}A}C_A(t) \qquad (6)\end{aligned}$$

$$\dot{C}_{k_{Br}}(t) = -iE_{k_{Br}}C_{k_{Br}}(t) - i\sum_{q=\uparrow,\downarrow}\sum_{k_{Br}} V_{k_{Br}k_{bq}}C_{k_{bq}}(t) \quad (7)$$

$$\dot{C}_{k_L}(t) = -iE_{k_L}C_{k_L}(t) - iV_{k_LD}C_D(t) \quad (8)$$

$$\dot{C}_{k_R}(t) = -iE_{k_R}C_{k_R}(t) - iV_{k_RA}C_A(t) \quad (9)$$

To get steady state formalism, we define $C_j(t)$ as $C_j(t) = \bar{C}_j e^{-iEt}$ with E represents the system eigen values. So we put$\dot{\bar{C}}_j = 0$ and by consider the following separation procedure:

$$V_{k_i\alpha} = v_{ki}V^{I\alpha} \qquad (10)$$

$$\bar{C}_{ki} = v_{ki}\bar{\bar{C}}_I \qquad (11)$$

With α=*A, D, Br* and *b*

by substituting these definitions in eqs.((4)-(9)) we obtain obvious expression for,

$$\bar{C}_A(E) = \frac{X_1(E)}{X_2(E)}\bar{C}_D(E) \qquad (12)$$

Where,

$$\begin{aligned}X_1(E) = \Bigg\{&\sum_{q=\uparrow,\downarrow} V^{Abq}\Gamma_{bq}(E)V^{bqD} + \\ &\Gamma_{Br}(E)\sum_{q=\uparrow,\downarrow} V^{Abq}\Gamma_{bq}V^{bqBr}\sum_{q=\uparrow,\downarrow} V^{Brbq}\Gamma_{bq}(E)\,V^{bqD}\Bigg\} \qquad (13)\end{aligned}$$

and,

$$\begin{aligned}X_2(E) = &\left\{E - E_A - \sum_{AR}(E) - \sum_{q=\uparrow,\downarrow}\sum_{Abq}(E)\right\}\times \\ &\left[1 - \Gamma_{Br}(E)\sum_{q=\uparrow,\downarrow}\sum_{Brbq}(E)\right] - \Gamma_{Br}(E)\left|\sum_{q=\uparrow,\downarrow} V^{Abq}\Gamma_{bq}(E)V^{bqBr}\right|^2 \qquad (14)\end{aligned}$$

Where,

$$\sum_{ij}(E) = \left|V^{ij}\right|^2\Gamma_j(E) \qquad (15)$$

represents the interaction self-energy, with[8],

$$\Gamma_j(E) = -i\pi\rho_j(E) + P\int \rho_j(E')dE'/(E - E') \qquad (16)$$

Where $\rho_j(E)$ is the electronic density of states of the subsystem j [9],

$$\rho_j(E) = \sum_{k_j}\left|v_{k_j}\right|^2\delta\left(E_{k_j} - E\right) \qquad (17)$$

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

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)} = \frac{X_1(E)}{X_2(E)} \qquad (18)$$

and,

$$T(E) = |t(E)|^2 \qquad (19)$$

Notably, in the following, the transmission spectrum will be calculated with E_A is fixed at 0.0.

2.2 The Case of Active Region contains the base pairs with backbones

In this section, we denote the active region which includes the DNA bases with the backbone by Br. Accordingly, we describe the system under study by using the following time–independent Hamiltonian, which takes into account all the sub-systems interactions by using Dirac's notations:

$$\hat{H} = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_{k_L} E_{k_L}|k_L\rangle\langle k_L| + \sum_{k_R} E_{k_R}|k_R\rangle\langle k_R| + \sum_{k_{Br}} E_{k_{Br}}|k_{Br}\rangle\langle k_{Br}| + \sum_{k_{Br}} [(V_{Dk_{Br}}|D\rangle\langle k_{Br}| + h.c) + (V_{Ak_{Br}}|A\rangle\langle k_{Br}| + h.c)] + \sum_{k_R} (V_{Ak_R}|A\rangle\langle k_R| + h.c) + \sum_{k_L} (V_{Dk_L}|D\rangle\langle k_L| + h.c) \quad (20)$$

The different indices D, A, Br, L and R denote donor, acceptor, DNA bases with the backbone, left lead and right lead respectively.

The system wave function can be written as,

$$\psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_{k_{Br}} C_{k_{Br}}(t)|k_{Br}\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle \quad (21)$$

By following the same procedure that over mentioned in section (2), we get:

$$\bar{C}_A(E) = \frac{X_1(E)}{X_2(E)}\bar{C}_D(E) \quad (22)$$

Where,

$$X_1(E) = V^{ABr}\Gamma_{Br}(E)V^{BrD} \quad (23)$$

$$X_2(E) = E - E_A - \sum_{AR}(E) - \sum_{ABr}(E) \quad (24)$$

Equations (23) and (24) are required to calculate the transmission probability for the case of scattering region containing the base pairs with backbones.

3. Results and Discussion

3.1The Case of Base Pairs Only

We will calculate the eigen values of the base pairs (for the arrangement of base pairs shown in fig.(1) which is also of homogenous sequence) by using tight binding model [10],

$$E_j = E_{basis} - 2tcos\left(\frac{\pi j}{N+1}\right) \quad (25)$$

Where, E_{basis} $(=(E_G+E_C)/2-t_{gc})$is the energy of the basis (i.e. the energy of one base pair), t_{GC} $(=0.04\ eV)$ is the hoping integral[10]. The energy levels positions in this case are lying in the range $1.50\ eV \le E \le 3.03\ eV$, within the LUMO levels with respect to lead Fermi level E_F=-5.5 eV.

Accordingly, the active region density of states is written as,

$$\rho(E_j) = \frac{N}{2\pi}\frac{1}{2|t|\ sin\ (\frac{\pi j}{N+1})} \quad (26)$$

The relationship between the transmission probability *T(E)* and energy E assuming the ladder model for the case belong to the active region contains the DNA bases only is illustrated in fig.(2) , where all energies are measured with respect to E_F=-5.5 eV . The peak-dip transmission number is also N-1, which is attributed to the interference effects. In all figures, it is obvious that each transmission spectrum experiences a quantum shift towards the higher energies. The connection up-up results in a high transmission probability as compared with the down-down connection because $V^{buD}>V^{bdD}$ and $V^{buA}<V^{bdA}$.

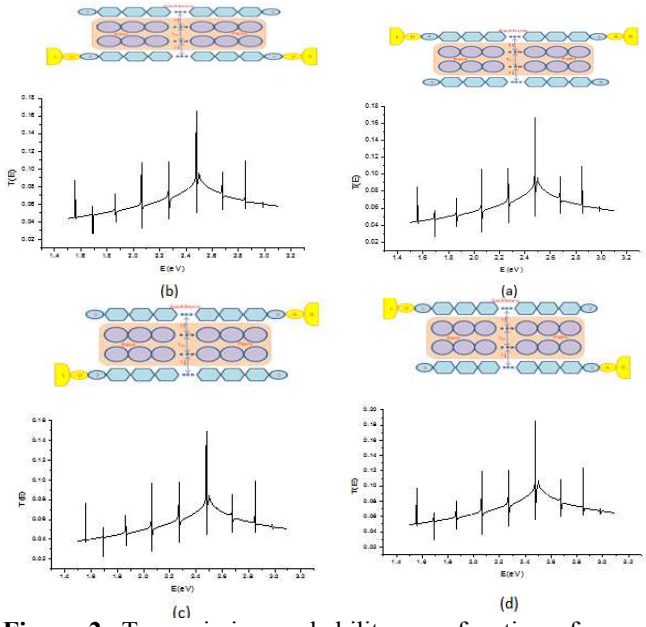


Figure 2: Transmission probability as a function of energy with sequence (G/C)10 and connections as (a) Doner-5-DNA-3-Accepter (b) Doner-3-DNA-5-Accepter (c) Doner-5-DNA-5-Accepter (d) Doner-3-DNA-3-Accepter for ladder model without backbone Parameters:V^{bu} =-0.7, V^{bd}=-0.65, V^{Abu}=-0.9, V^{Abd} = -0.85, V^{buD} =0.85, V^{bdD} =-0.85, t_{12} =0.04 and *t*=-0.4 are all in eV.

3.2 The Case of Base Pairs with Backbone

We calculate the eigen values of the bridges (base pairs with backbone) by using tight binding model [11],

$$E_j = E_{basis} + \frac{1}{2}\left(-t_{12} - 2tcos\left(\frac{\pi j}{N+1}\right)\right) \pm \frac{1}{2}\sqrt{(t_{12+}t\ cos\left(\frac{\pi j}{N+1}\right))^2 + 4t_{\uparrow,\downarrow}^2} \quad (27)$$

Where, t_{12} is the strength of hydrogen bond, $t_{12}=0.04\ eV$. The energy levels positions in this case are lying in the range $0.32\ eV \le E \le 1.29\ eV$, which are lying in the LUMO levels. Accordingly, we write the scattering region density of states as,

$$\rho(E_j) = \frac{N}{2\pi}\frac{\sqrt{(t_{12} + t\ cos\left(\frac{\pi j}{N+1}\right))^2 + 4t_{\uparrow,\downarrow}^2}}{2tsin\left(\frac{\pi j}{N+1}\right)\left(\sqrt{(t_{12} + t\ cos\left(\frac{\pi j}{N+1}\right))^2 + 4t_{\uparrow,\downarrow}^2} + t_{12} + 2tcos\left(\frac{\pi j}{N+1}\right)\right)} \quad (28)$$

Our calculations for the case assuming the ladder model with backbones are illustrated in fig.(3). The peak-dip transmission behavior emerge for $E > 1.6\ eV$. The width of the resonances is not equal because the energy levels at which the electrons can hop are not the same along the active region. It is obvious that the transmission spectrum is shifted in the energy axis toward the higher energies.

Finally, the values of *T(E)* is determined by the system eigen values, the coupling interaction between subsystems and the number of channels for the electron to transfer.

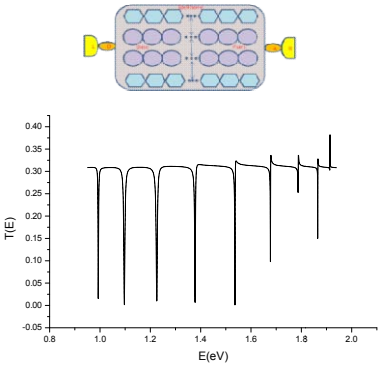


Figure 3: Transmission probability as a function of energy with sequence (G/C)10 and connection as Doner--DNA--Accepter for ladder model with backbone Parameters: V^{bu} =-0.7, V^{bd}=-0.7, V^{ABr} =-0.9, V^{BrD} =-0.5and t=-0.4 are all in eV.

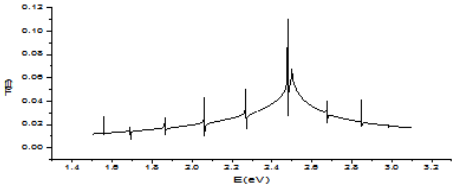
3.3 The Strong Coupling Limit

The probability of transmission in the relatively strong coupling (between the base pairs and backbones) limit is investigating and studied in this section. Experimentally, changing the coupling strength with the backbones corresponds to the environmental changes.

Due to relatively small values of the electronic coupling (between base pairs) parameters, the eigenvalues are lying very close to the onsite energies of the respective active region (see figs.((4)-(5)). Changing the coupling strength in the backbone correspond experimentally to the environment changes.

The probability of transmission shows strong dependence on the DNA-lead coupling strength, so a series of N-1 well defined transmission resonances appear. This regime is called the resonant tunneling regime where the resonances correspond to the energies of the electronic states confined in the active region (*i.e.* molecular wire of N sites). For strong coupling limit one may expect that the electronic structure is modified significantly, which leads to resonances shifted and broadened.

It is obvious in our calculations that there is noticeable reduction in the values of transmission probability; this change comprises all the range of energy. It is well known that the determination of the hybridization interactions is not so simple problem and it must be related to the motive which may be physical, chemical or biological.



(a)

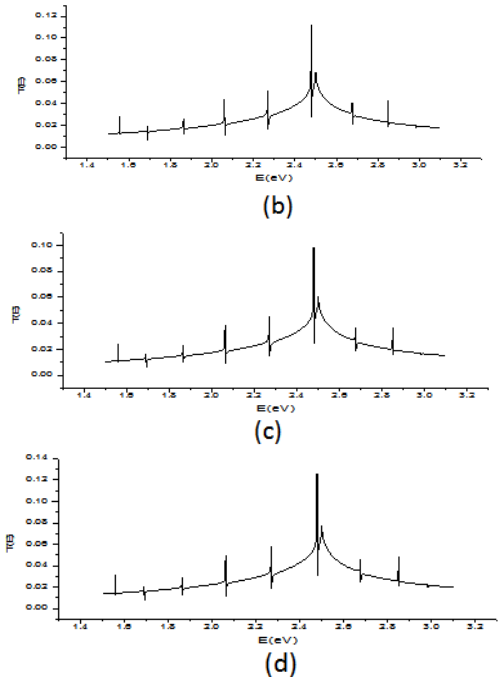


Figure 4: Transmission probability as a function of energy with sequence (G/C)10 and connection as Doner-5-DNA-3-Accepter for ladder model without backbone. Parameters: V^{bu} =-1.4, V^{bd} =-1.3, V^{Abu}=- 0.9, V^{Abd} =-0.85, V^{buD} =-0.9, V^{bdD} =-0.85 ,t_{12} =0.04 and t=-0.4 all are in eV.

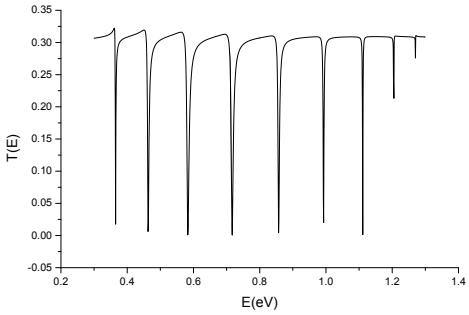


Figure 5: Transmission probability as a function of energy with sequence (G/C)10 and connection as Doner--DNA--Accepter for Ladder model with backbone Parameters: V^{bu}=V^{bd}=-1.4 , V^{ABr} =-0.9, V^{BrD} =-0.5, t=-0.4 are all in eV.

3.4The Tunneling Current Calculation

It is well known that the calculating of the transmission spectrum is the most important step in studying the transport and dynamic properties of the electron transport process in nanostructures.

In this section, our transmission spectrum calculations will be employed to calculate the electric current through the DNA molecule.

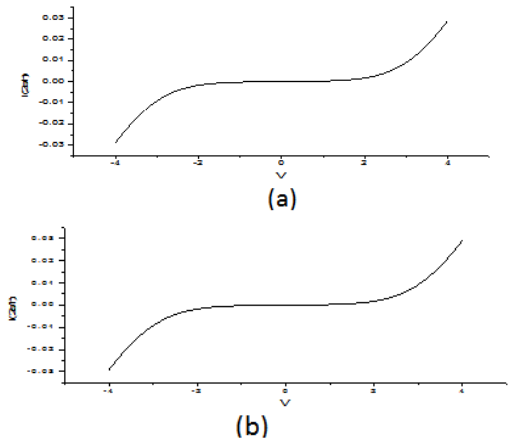
The electric current through the active region (base pairs with or without backbone) can be calculated by using the Landauer transport formula [12-13]:

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_L(E) - f_R(E)]dE \qquad (29)$$

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

$$f_\alpha(E) = \left\{1 + exp\left[\frac{E-\mu_\alpha}{K_B T_\alpha}\right]\right\}^{-1} \quad (30)$$

$\mu_\alpha$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, which means that the leads are in thermal equilibrium. The tunneling current properties are investigated by sweeping 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 figs.((6)-(7)). The *I-V*curves clearly show a nonlinear dependence. From these figures, we can clearly identify two regimes. In the first, the current is vanished for certain range of bias voltage as shown in table(1) which summarizes all information about the ladder model for two cases (with and without backbones). This voltage gap is type connection-dependent. All Figures illustrate that the DNA acts as an insulator in low voltage bias. At relatively higher bias voltages, the current shows a drastic increase as shown in all figures. The difference in voltage gap may be attributed to the difference in resistance which is type connection-dependent. Also notable is the fact that the *I-V* characteristics are approximately symmetric with respect to the absolute value of the bias polarity, since the active region is placed in the middle of the gap between the electrodes. In general, the currents through the active region with backbone are found to be higher than the calculated current for the active region without backbone. Our results represent a good qualitative agreement with the electronic structure (*i.e.* the transmission spectrum) of the system along the zero current part of the *I-V* curves. The observed voltage gap in the *I–V* characteristics cannot be directly related with the HOMO-LUMO gap of our DNA molecules.



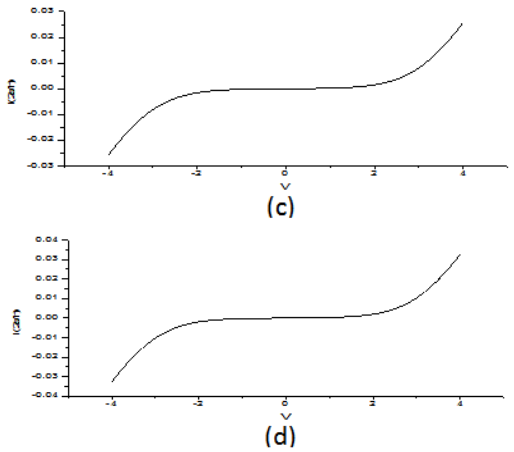


Figure6: Current as a function of bias voltage with sequence (G/C)10 for ladder model without backbone. Parameters: V^{Abu}=- *0.9,* V^{Abd} *=-0.85,* V^{buD} *=-0.9,* V^{bdD} *=-0.85,* V^{bu} *=-0.7,* V^{bd}*=-0.65,* t_{12}*=0.04 and t=-0.4 all are in eV.*

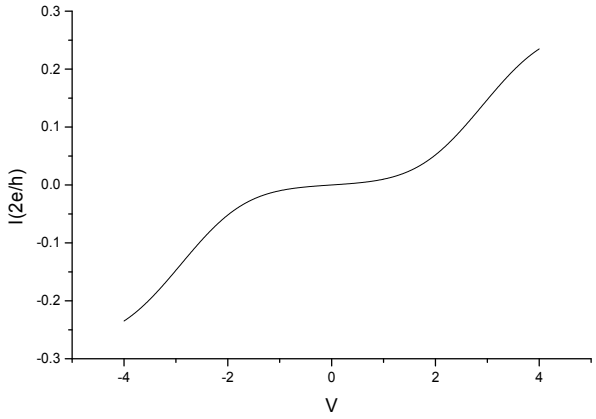


Figure 7: Current as a function of bias voltage with sequence (G/C)10 for ladder model with backbone. Parameters: $V^{bu}=V^{bd}$*=-0.7,* V^{ABr} *=-0.9,* V^{BrD} *=-0.5, t=-0.4 and* t_{12}*=0.04* all are in*eV.*

The values of voltage gap may also strongly depend on the disorder and correlation which are not included in our work.

Table 1: Represents the values of voltage gap for the ladder model for two cases (with and without backbones).

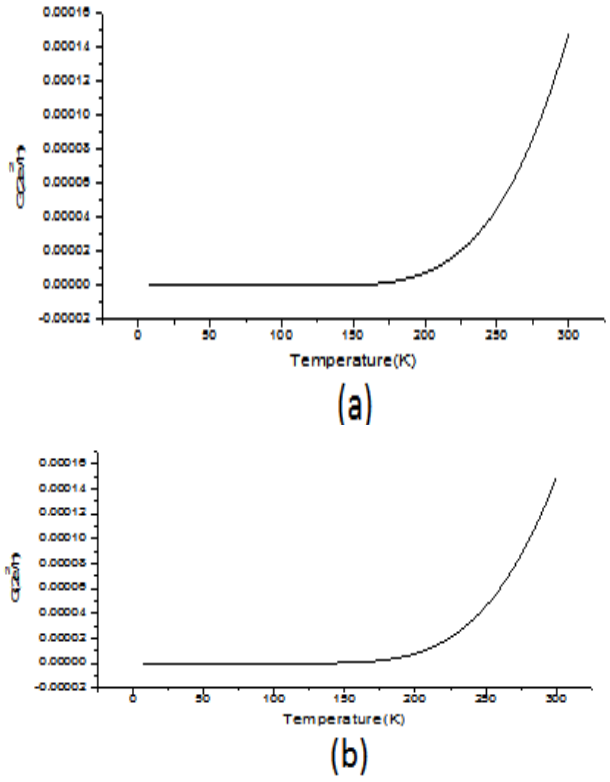
Model	Type of Connection	Voltage gap (eV)
Ladder model Without backbone	Up-up	1.1
	Down-down	1.1
	Up-down	1.2
	Down-up	1.02
Ladder model With backbone	----------	0.02

3.5 Conductance Calculations

In this section 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. We will summarize our results for the conductance, as long as the transmission probability is obtainable in our model calculation, by using the following formula [14],

$$G = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\, T(E)\frac{\partial f(E)}{\partial E} \qquad (31)$$

With *f(E)* is defined in eq(27). As the thermal equilibrium is considered in our calculation $T_R=T_L=T$ with $0 < T < 300$ *K*. Our results presented in fig.(8) is with base pairs only in the case of ladder model. While fig.(9) represents our calculation with base pairs and backbones in the case of ladder model. One can observe that the conductance is independent on temperature for $0 < T < 150$ *K*, we note that the conductance stays constant with increasing of temperature until it reaches nearly *150 K*. While it is nonlinear for $T > 150$ *K*, one can observe high and sudden increasing in the conductance with normal increasing of temperature. This may attributed to the thermal broadening of the Fermi function, since our treatment does not include effects of molecular vibrations. It is too difficult to explain the observed temperature dependence in DNA. According to our treatment, the strong conductance – temperature dependence at relatively high temperatures can be attributed to the increase in the hybridization between the active region energy levels with the left and right leads levels as the temperature increases. For $T > 150$ *K*, one can assume that the conductance is enhanced by the hopping transport mechanism between the chemical potentials and active region energy levels that lying above the chemical potential and then between adjacent sites.



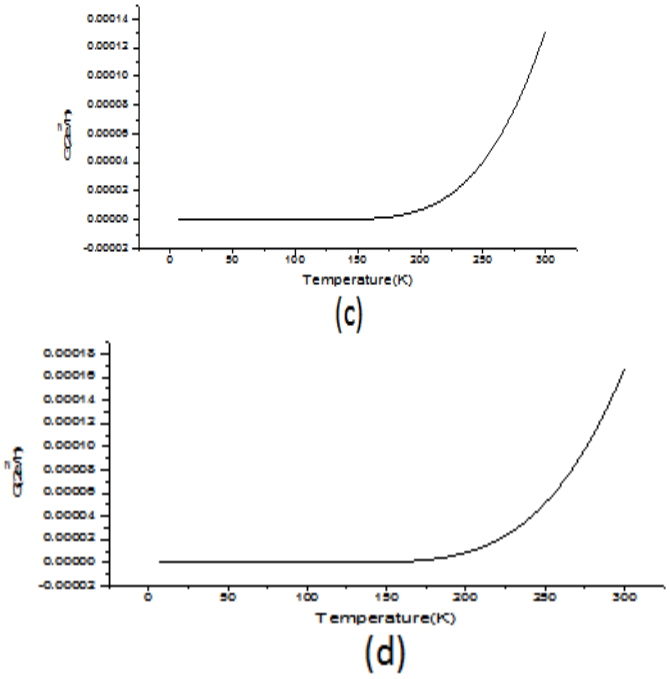


Figure 8: Conductance as a function of temperature with sequence (G/C)10 and connections as (a) Donor-5-DNA-3-Accepter and (b)Donor-3-DNA-5-Accepter (c) Donor-3-DNA-3-Accepter and (d)Donor-5-DNA-5-Accepter for ladder model without backbone with Parameters: *t=-0.4,* V^{bu} *= -0.7,* V^{bd}*= -0.65,* V^{Abu}*=-0.9,* V^{Abd}*=-0.85,* V^{Dbu}*=-0.9,* V^{Dbd}*=-0.85,* t_{12}*=0.04 in eV.*

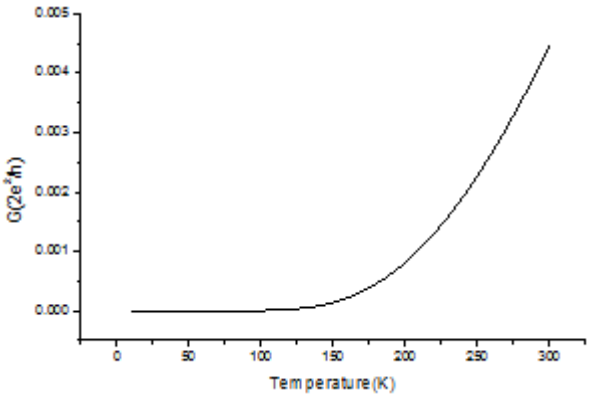


Figure 9: Conductance as a function of temperature with sequence (G/C)10 for ladder model with backbone with Parameters: *t=-0.4,* $V^{bu}=V^{bd}$*=0.7,* V^{Abu}*=-0.5,* V^{ABr}*=-0.9,*V^{BrD}*=-0.5 and* t_{12}*=0.04 in eV.*

Notably, it is obvious that the conductance behavior is the same for all types of connection. At T=300K, the values of conductance are determined by the types of connection for the calculations that are performed for the base pairs only in the case of ladder model (see table (2)). For the up-up connection, the conductance for the ladder model. Experimentally [15] the temperature dependent conductivity is explained by suggesting two transport mechanisms, i.e. ionic conduction at low temperatures and temperature driven hopping transport processes at high temperatures. The underlying physics of the weak temperature dependence at low temperatures was not understood.

Table 2: The conductance G (in unit of $(2e^2/h)$) for the ladder model at two different temperature with different connecting, for the sequence (G/C)10.

Model	Type Connection	G at 50 K	G at 300 K
Ladder model without Backbone	Up-up	3.14×10^{-17}	1.48×10^{-4}
	Down-down	3.18×10^{-17}	1.49×10^{-5}
	Up-down	2.80×10^{-17}	1.32×10^{-4}
	Down-up	3.57×10^{-17}	1.67×10^{-4}
Ladder model with Backbone	----------	9.64×10^{-11}	0.00741

4. Conclusions

In this paper, different results about charge transport in DNA system are reviewed. DNA conductivity depends on conditions like number of base pairs, base pairs sequences, temperature, and contact to electrodes and so on. According to different sets of results that DNA molecules behave like insulator, semiconductor and conductor. The transport through DNA in molecular junctions demonstrated the ability to control the connectivity between the double strand and the two electrodes. Interestingly, no significant difference was determined between the conductances when using different connection strategies [16] for a homogenous DNA sequence. In contrast, our calculations of currents through an ordered sequence showed high values of magnitude suggesting that for such ordered sequences. Based on our reduced contact probabilities analysis those show those such transport through ordered sequences are sensitive to the connection strategy. Theoretical evaluation of the current requires explicit account for many effects including coupling to electronic interactions that were excluded in the present treatment. The transport through transient structures, associated with temporal fluctuations in the tight-binding model parameters. Some significant electronic conduction properties for DNA molecule in the donor/DNA/accepter system have been studied by using ladder model. Our results suggest a good agreement with the electronic structure of the DNA in the ladder, additional we have presented a technique that allows the computation of electron transport through short sequences of DNA, including transmission probability, *I-V* characteristics and temperature dependent conductance.

References

[1] D. D. Eley and D. I. Spivey, Trans. Faraday Soc. 58, 411 (1962).
[2] S. O. Kelley and J. K. Barton, Science 283, 375 (1999).
[3] K. Keren, R. S. Berman, E. Buchstab, U. Sivan, and E. Braun, Science 302,1380 (2003).
[4] M. Mertig, R. Kirsch, W. Pompe, and H. Engelhardt, Eur. Phys. J. D 9, 45 (1999).
[5] B. Xu, P. Zhang, X. Li, and N. Tao, Nano Lett.4, 1105 (2004).
[6] N. R¨osch and A. A. Voityuk, Top. curr. chem. 237, 37 (2004).
[7] F. M. Izrailev and A. A. Krokhin, Phys. Rev. Lett. 82, 4062 (1999).
[8] G. Sedghi, V. M. Garcia-Suarez, L. J. Esdaile, H. L. Aderson, C. J. Lambert, S.Martin, D. Bethell, S. J. Higgins,M. Elliott, N. Bennett, J. E. Macdonald, and R. J. Nichols, Nature Nanotechnology 6, 517 (2011).
[9] M.A. Ratner, J. Phys. Chem. 94, 4877 (1990).
[10] P. W. Anderson, Phys. Rev. 109, 1492 (1958).
[11] D. K. Klotsa, R. A. R¨omer, and M. S. Turner, Biophys. J. 89, 2187 (2005).
[12] R. Landauer, Philos. Mag. 21, 863 (1970).
[13] M. Buttiker, Phys. Rev. B 35, 4123 (1987).
[14] Natallia V. Grib, Dmitry A. Ryndyk, Rafael Gutiérrez, GianaurelioCuniberti, Journal of Biophysical Chemistry, Vol.1, No.2, 77-85 (2010).
[15] Guo, X.; Gorodetsky, A. A.; Hone, J.; Barton, J. K.; Nuckolls, C. *Nat. Nanotechnol.3*, 163–167 (2008).