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Modeling of electron localization in a quasi-one-dimensional tight-binding chain

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المستخلص

نمذجة تموضع الكترون شديد التقيد في بعد واحد لشبه سلسلة, في هذا البحث نقدم صيغة رياضية عامة لاحتمالية انتقال الكترون خلال جزيئات الدي ان اي حيث تم اشتقاقها في مستوى حجم النانوميتر وذلك بافتراض ان جزيئات الدي ان اي كسلسلة نانووسلك تشبه نموذج عظم السمكة .درسنا احتمالية تموضع نوعين من الدي ان اي المتتابع وهما وشخصت الانتقالات خلال هذه الدوريات وكلاهما عند درجة حرارة من 0 الى 300 كلفن وهذه الدراسة تضمنت استقصاء وتركيز على [(A/T)10] and [(G/C)10] تلك الدوريتين .

Abstract

In this paper we propose general formula for the transmission probability for electron transfer through DNA molecules have been derived in the level of nanometers size , by assuming DNA molecules chain as nano wire. We studied localization properties for two DNA sequences: [(G/C)10] and [(A/T)10]. We have also investigated and focused on the transmission for the these two periodic ,and both at temperature degrees (0 and 300K).

Keywards; transmission, localization, DNA.

Introduction

The concept of localization comes in to help in understanding strong disorder. Localization is a wave property. Electromagnetic waves, water waves or particle waves all can display localization. The phenomena of localization exist when waves interact with disordered mediums. The localization of an electron implies that its wave function vanishes exponentially away from the center of localization. The localization length is the measure of the spatial extension of the localized state. If the localization length considerably exceeds all other relevant lengths in the system (size of the system, mean-free

path etc.), then the electron can extend to infinity and contribute to electron transport. If localization length is smaller in comparison to the system length, the particles occupying those states do not interact with the boundaries, thus they do not contribute to electron transport[1]. The popular model for electronic transport in DNA is considered in this paper, the Fishbone model. It is based on tight-binding single electron Hamiltonians [2, 3]. In the Fishbone model of DNA, electron transport in a DNA molecule is considered as discrete jumps between the neighboring base nucleotides. Due to strong A-T and C-G coupling, it is usually considered that there is a single electron channel with a binary sequence of the on-site potentials with energies $\varepsilon_{A\text{-}T}$ = 8.69 eV and $\varepsilon_{G\text{-}C}$ = 8.31 eV. These on-site energies are taken as the average of the ionization energies of the bases that form the base pair. The corresponding ionization energies are ε_A = 8.24 eV, ε_T = 9.14 eV, ε_C = 8.87 eV and ε_G = 7.75 eV. Each site (base pairs A-T and C-G) in this sequence has a link to the backbone structure, see Fig.(1). From the base site an electron may jump either to the neighboring sites or to one of the backbone [4, 5].

Definition of the problem

The first case, considered in this paper, is the case of fishbone model that illustrated as below.

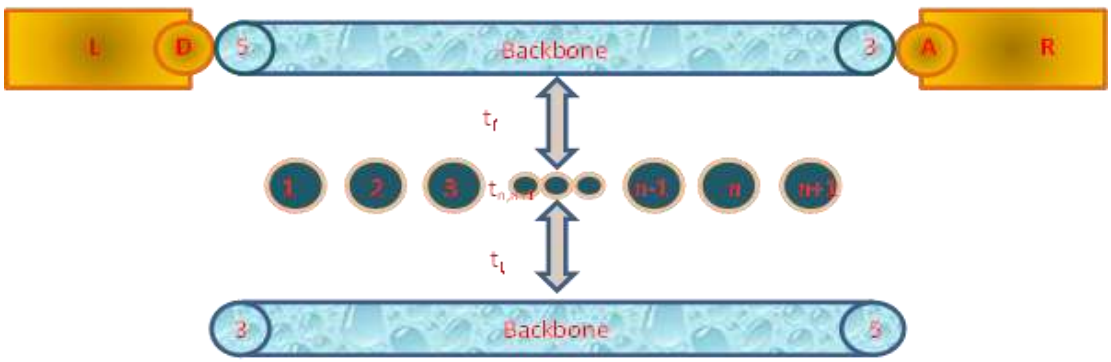

Fig.(1) A schematic illustration for the fishbone model.

Each base pair is considered as one active region while the effects of backbones are incorporated in the coupling interactions with each base site.

The total number of the active regions equals N. Each active region has energy sites equals to E_n with n=1,2,3,…….N.

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

$$\hat{H} = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_n E_n\,|n\rangle\langle n| + \sum_{k_L} E_{k_L}\,|k_L\rangle\langle k_L| + \sum_{k_R} E_{k_R}\,|k_R\rangle\langle k_R| + \sum_{q=\uparrow,\downarrow}\sum_{k_{bq}} E_{k_{bq}}\,|k_{bq}\rangle\langle k_{bq}| + \sum_{n=1}^{N}[V_{n,n+1}\,|n\rangle\langle n+1| + H.C.] + \sum_{q=\uparrow,\downarrow}\sum_n\left\{\sum_{k_{bq}}\left[V_{k_{bq}n}|k_{bq}\rangle\langle n\right|\right.$$

$$\left. + H.C.]\right\} + \sum_{q=\uparrow,\downarrow}\sum_{k_{bq}}\left[(V_{Dk_{bq}}|D\rangle\langle k_{bq}| + H.C.) + (V_{Ak_{bq}}|A\rangle\langle k_{bq}| + H.C.)\right] + \sum_{k_L}[V_{Dk_L}|D\rangle\langle k_L| + H.C.] + \sum_{k_R}[V_{Ak_R}|A\rangle\langle k_R| + H.C.] \quad \ldots (1)$$

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

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

The index k_j is the energy wave vector. The equation of motion for $C_j(t)$ can be obtained by using Schrodinger equation(in atomic unit),[6]

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

The equations of motion for $C_j(t)$ can be obtained by using time dependent Schrodinger equation ,

With A_{bq} is given by,[7]

$$A_{bq}(E) = \sum_{k_{bq}} \left|V_{k_{bq}}\right|^2 \bar{\bar{C}}_{bq} = \Gamma_{bq}(E)\left\{V^{bqD}\bar{C}_D(E) + V^{bqA}\bar{C}_A(E) + \sum_n V^{bqn}\bar{C}_n(E)\right\} \quad (4)$$

Now we define,

$$\left.\begin{aligned} a_{bqn}(E) &= \Gamma_{bq}(E)V^{bqn} \\ b_{bqn}(E) &= \Gamma_n(E)V^{nbq} \\ d_{nm}(E) &= \Gamma_n(E)V_{nm} \end{aligned}\right\} \quad (5)$$

$\Gamma_i(E)$ is defined by eq.(2.22) with i=bq,n. And,

$$g_{bq}(E) = \Gamma_{bq}(E)\{V^{bqD}\bar{C}_D(E) + V^{bqA}\bar{C}_A(E)\} \quad (6)$$

Then, equations (3.20) and (3.22) are rewritten as follows,

$$b_{bqn}(E)A_{bq}(E) - \bar{C}_n(E) + \sum_{m\neq n} d_{nm}(E)\bar{C}_m(E) = 0 \quad (7)$$

$$A_{bq}(E) - \sum_{n} a_{bqn}(E)\bar{C}_n(E) = g_{bq}(E) \quad (8)$$

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

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

In order to solve the system of the over-mentioned related equations, we construct the following matrix-form equation,

$$\begin{vmatrix} -1 & a_2 & a_3 & a_4 & \bullet\bullet\bullet & a_{n-1} & a_n \\ b_{b\uparrow 1} & -1 & d_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 2} & d_{21} & -1 & d_{23} & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 3} & 0 & d_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ b_{b\uparrow n-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & d_{n-2,n-1} \\ b_{b\uparrow n} & 0 & 0 & 0 & \bullet\bullet\bullet & d_{n-1,n-2} & -1 \end{vmatrix} \begin{vmatrix} A_{b\uparrow} \\ \bar{C}_1 \\ \bar{C}_2 \\ \bar{C}_3 \\ \bullet \\ \bullet \\ \bar{C}_{n-2} \\ \bar{C}_{n-1} \end{vmatrix} = \begin{vmatrix} -g_{b\uparrow} \\ 0 \\ 0 \\ 0 \\ \bullet \\ \bullet \\ 0 \\ 0 \end{vmatrix}$$

Then, by defining,

$$\Delta_{\uparrow} = \begin{vmatrix} -1 & a_2 & a_3 & a_4 & \bullet\bullet\bullet & a_{n-1} & a_n \\ b_{b\uparrow 1} & -1 & d_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 2} & d_{21} & -1 & d_{23} & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 3} & 0 & d_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ b_{b\uparrow n-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & d_{n-2,n-1} \\ b_{b\uparrow n} & 0 & 0 & 0 & \bullet\bullet\bullet & d_{n-1,n-2} & -1 \end{vmatrix}$$

and,

$$\Delta_{a\uparrow} = \begin{vmatrix} -1 & a_2 & a_3 & a_4 & \bullet\bullet\bullet & a_{n-1} & a_n \\ b_{b\uparrow 1} & -1 & d_{12} & 0 & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 2} & d_{21} & -1 & d_{23} & \bullet\bullet\bullet & 0 & 0 \\ b_{b\uparrow 3} & 0 & d_{32} & -1 & \bullet\bullet\bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet\bullet\bullet & \bullet & \bullet \\ b_{b\uparrow n-1} & 0 & 0 & 0 & \bullet\bullet\bullet & -1 & d_{n-2,n-1} \\ b_{b\uparrow n} & 0 & 0 & 0 & \bullet\bullet\bullet & d_{n-1,n-2} & -1 \end{vmatrix}$$

Notably, each element in equations (10-12) is a function of energy but it is not shown for simplicity. Now we rewrite equation(9) in the following form ,

$$\bar{C}_A(E) = \frac{V^{Ab\uparrow}\Delta_{a\uparrow 01}(E)}{(E - E_A - \sum_{AR}(E))\Delta(E) - V^{Ab\uparrow}\Delta_{a\uparrow 10}(E)}\bar{C}_D(E) \qquad (13)$$

Where,

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

(14)

represents the interaction self-energy ,with ,

$$\Gamma_j(E) = -i\pi\rho_j(E) + P\int \rho_j(E')dE'/(E - E') \qquad (15)$$

and

$$\rho_j(E) = \sum_{k_i} |v_{k_i}|^2 \delta(E_{k_i} - E) \quad (16)$$

With $k_i=k_L$, k_R , k_{Br} and k_b .Where $\rho_i(E)$ is the electronic density of states of the subsystem i.

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

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)} \quad (17)$$

and ,

$$T(E) = |t(E)|^2 \quad (18)$$

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. Fig.(2-3) show two plots of the transmission coefficient as a function of electron energy at 0 K and 300 K 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. It is clearly seen that as temperature is increased from 0 K to 300 K, the resonant peaks, which initially had unit transmission, become suppressed and smear out below unity due to the random variation of the hopping integrals. We observed that the resonant peaks have increased at high temperature (300K) because of many states get sufficient energy to hop from valance band to conductance band. As well, can observe 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, become suppressed and smear out below unity due to the decrease in the number of transmitting states, while the resonance positions are shifted due to the phase changes of the electrons. A

DNA double helix with disoriented base-pairs due to the thermal fluctuations can be viewed as a quasi-one-dimension disordered system.

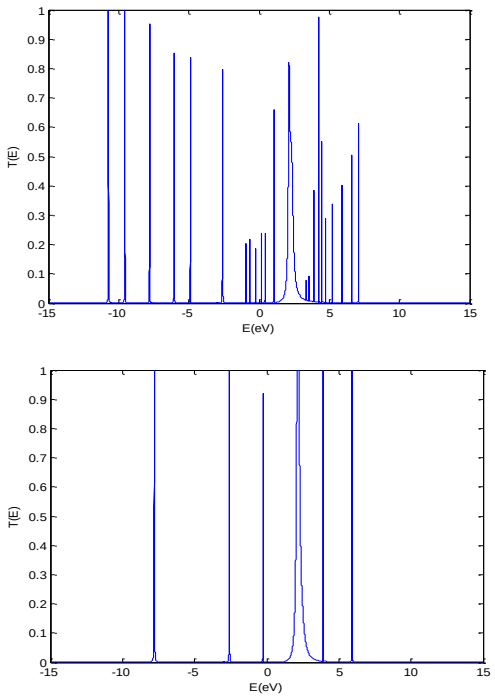

Fig.(2) Transmission probability as a function of energy at temperature is (a) (0K) and (b) (300K) with sequence (G/C)10 and connections as Donor-5-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5, V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

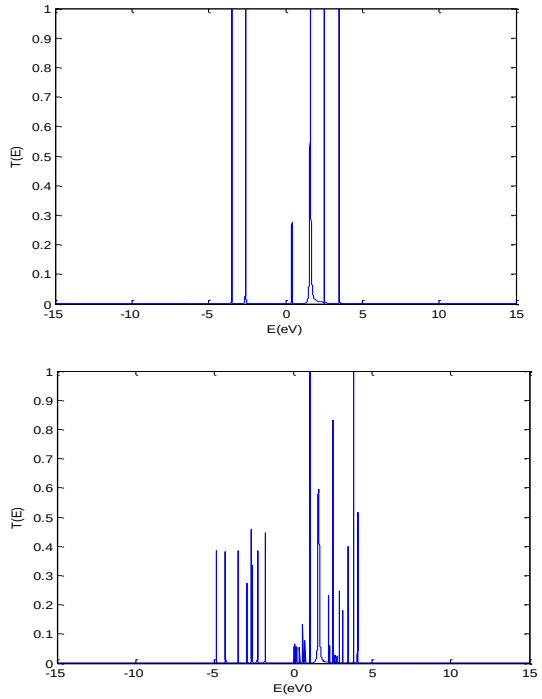

Fig.(3) Transmission probability as a function of energy at temperature is (a) (0K) and (b) (300K) with sequence (A/T)10 and connections as Donor-5-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=-0.5, V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

We also show the localization length as a function of electron energy for two different temperatures, 0K and 300K, in Figs.(4-5) 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. To address the effects of thermal structural fluctuations on electron localization, we plot the localization length as a function of electron energy for two different temperatures, T =0 K and T = 300 K. High temperature leads to the disorder of the system and a reduction of the localization length and consequently a reduction of the electron conductance. Notice that the magnitude of the localization length of (G/C) sequence at T = 0 K is approximately 4 times larger than that at T = 300 K while the magnitude of the localization length of (A/T) sequence at T = 0 K is approximately 120 times larger than that at T = 300 K. This clearly indicates

that thermal structural fluctuations localize the electronic wave functions, resulting in a temperature-dependent localization length.

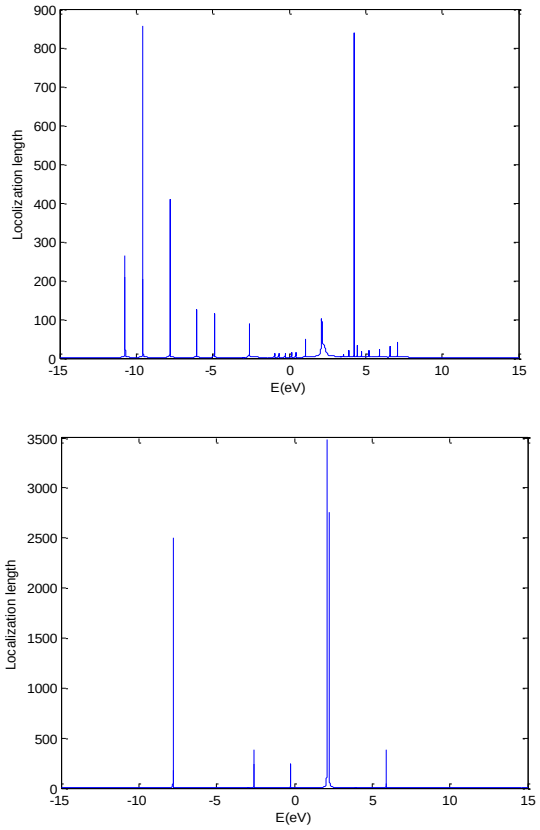

Fig.(4) Localization length as a function of energy at temperature is (a) (0K) and (b) (300K) with sequence (G/C)10 and connections as Donor-5-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.5,V^{Abd} =-0.75, V^{buD} =-0.75, V^{bdD} =-0.5 , $t_{\uparrow}$=-0.7, $t_{\downarrow}$=-0.75 and t=-0.5 all are in eV.

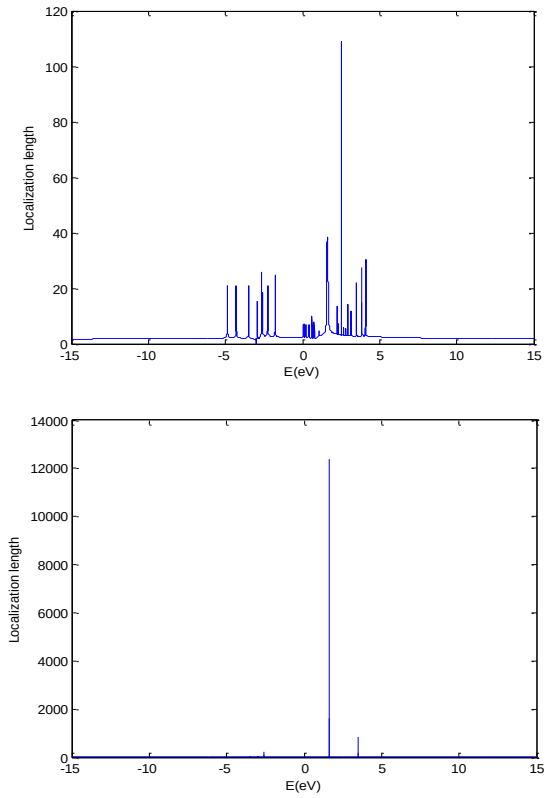

Fig.(5) Localization length as a function of energy at temperature is (a) (0K) and (b) (300K) with sequence (A/T)10 and connections as Donor-5-DNA-3-Accepter for fishbone model with Parameters: V^{Abu}=- 0.45,V^{Abd} =-0.7, V^{buD} =-0.7, V^{bdD} =-0.45 , $t_{\uparrow}$=-0.65, $t_{\downarrow}$=-0.45 and t=-0.25 all are in eV.

Conclusion

In this paper is a study of Anderson localization of electrons in one-dimension in DNA system. It also involves a computational part where the localization length is calculated for DNA system at (0K and 300K) temperature with two sequences are (G/C)10 and (A/T)10 . In this model the DNA is a one-dimensional wire (fishbone model). My work on electron localization in single-channel Fishbone model for DNA system shows that DNA system can have localized electron states depending on their genetic sequence information and temperature. The calculations give a link between the functionality of DNA regions and their electron localization properties.

Another important point of investigation for near future is to see whether small changes in the sequence lead to any change in the localization length.

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