



Electronic transport through renormalized DNA chains

Transporte electrónico a través de cadenas de ADN renormalizadas

García Flores Daniel¹, Iglesias Vázquez Priscilla Elizabeth¹, Villarreal Sánchez Rubén César^{1,2} 

¹Facultad de Ciencias, Universidad Autónoma de Baja California. Carretera Tijuana-Ensenada Km 106, 22800 Ensenada, Baja California, México

²Facultad de Ingeniería, Arquitectura y Diseño, Universidad Autónoma de Baja California. Carretera Tijuana-Ensenada Km 106, 22800 Ensenada, Baja California, México

Autor de correspondencia: Daniel García Flores, Facultad de Ingeniería, Arquitectura y Diseño Universidad Autónoma de Baja California. Carretera Tijuana-Ensenada Km 106, 22800 Ensenada, Baja California, México, daniel.garcia.flores@uabc.edu.mx

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Resumen. - *El ADN ha presentado a través de experimentos una gran variabilidad en términos de sus características electrónicas. Han demostrado que puede adquirir el comportamiento de un conductor, semiconductor o aislante, lo que lo convierte en un buen candidato para replicar en dispositivos electrónicos a escala mesoscópica. En el presente trabajo, el coeficiente de transmisión cuántica se calcula para cadenas de ADN de varias longitudes con el uso del procedimiento de diezmado y renormalización, dentro de la aproximación de unión estrecha y la teoría de dispersión de Lippmann-Schwinger. Se obtuvieron perfiles de transmisión de energía, lo que ayudó a inferir las propiedades de transporte electrónico del sistema. Además, también se calculó la relación corriente-voltaje para una cadena de 30 pares, y se comparó con los resultados experimentales de Porath et al. Los resultados muestran las características de los semiconductores de la molécula, y un parecido con el trabajo de Porath, mostrando la calidad del procedimiento y el modelo utilizado.*

Palabras clave: ADN; Transporte electrónico; Corriente eléctrica; Transmitancia.

Abstract. - *DNA have presented through experiments great variability in terms of its electronic characteristics. They have shown that it can acquire the behavior of a conductor, semiconductor or insulator, making it a good candidate for replicating at the mesoscopic scale electronic devices. In the present work, the quantum transmission coefficient is calculated for DNA chains of various lengths with the use of the decimation and renormalization procedure, within the tight binding approximation and the Lippmann-Schwinger scattering theory. Transmission-Energy profiles were obtained, which helped to infer electronic transport properties of the system. Additionally, the current-voltage relation for a 30-pairs chain was calculated as well, and compared with the experimental results of Porath et al. Results show the semiconductor characteristics of the molecule, and a resemblance with the work of Porath, showing the quality of the procedure and the model utilized.*

Keywords: DNA; Electronic transport; Electrical current; Transmittance.



1. Introducción

Deoxyribonucleic acid (DNA) is well known for being the molecule where life is codified. Advances in nanotechnology have opened opportunities to study more about the molecule in another context: as an electric component. Recent experiments have shown that DNA can emulate electronic components (conductor, semiconductor, insulator, etc.) at the mesoscopic scale, depending on the conditions the experiment and environment [1]; taking into account that the transport occurs in a monomodal way at the central chain of nitrogenous pair bases [2], making it a great candidate for molecular electronics.

DNA also provides complexity in its structure. To calculate electronic transport, we have simplified the problem by describing the system through effective parameters by the means of the Green Function technique [3] for the renormalization of it, with a model that will carry its electronic characteristics. We focus on finding the relation between the transmittance T —*i.e.*, the amount of ingoing charge versus the outgoing, and the induced energy E , to obtain $T(E)$ profiles. These profiles will help us to infer the electronic properties of the system. Additionally, we have calculated deformations in the system given an external factor, with the purpose of locating optimal energy intervals where transmittance keeps its maximum value, if the system is strained.

To see the effectiveness of the theoretical analysis, we also calculated the I - V curve and compared it with the experimental results of Porath *et al* [4], where they measured electrical current through DNA wires.

2. Methodology

For the purpose of simplifying the molecule and to obtain an analytical result—based on [3], we made use of the decimation and renormalization procedure within the tight binding approximation,

on a model that could interpret the behavior of the transport in the intern and outer column (of nitrogenous base pairs and sugar phosphates, respectively). The *fishbone* model (Figure 1), previously utilized [5], was chosen for this.

Here $\alpha_{1,4,7}$ represents the base pair atomic sites of the intern column, meanwhile $\alpha_{2, 3, \dots, 9}$ the sugar atomic energy sites of the outer. On the other hand, β_{ij} is the bond energy from the site i to the site j , taking into account the tight binding approximation to first neighbors. Terminals 1 and 2 are molecular, widely used in experiments [6]. From this the renormalization equations of the system can be obtained, with aid of the Lippmann-Schwinger equation transmittance T is calculated, that will yield $T(E)$ profiles, where electronic properties of the system can be identified, and later used to calculate current through it and compare with the experiment of Porath [4]. Porath *et al* measured current through a 10.4nm long, double-stranded poly(G)-poly(C) DNA molecule, which is about 30 base pairs; specific base pairs were not taken into account, just atomic energy sites.

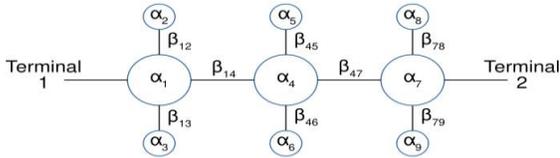


Figure 1. DNA’s fishbone model

2.1. Renormalization procedure

We start with the Greenian matrix (G_{mn}) version of the discretized Schrödinger equation, which takes the form:

$$(E - \alpha_m)G_{mn} = \delta_{mn} + \sum_k \beta_{mk}G_{kn} \quad (1)$$

where E is the energy, $\alpha_m(\beta_{mk})$ are the atomic energy site m (bond energy from site m to site k), δ_{mn} is the Kronecker delta, and G_{kn} the Green function given the points k, n . The problem is



solved in parts; first the particular equation for a base pair and its respective sugars, and then the junction of renormalized sites to form effective dimers. The proposed model for the particular case of a base pair can be seen in Figure 2, where the superscripts z and b tag whether it is a sugar or a base, respectively. Expanding (1) for the 1, 2 and 3 considered molecule sites, we obtain:

$$\alpha = \alpha + \beta^{(z)2} \quad (2)$$

where α represents the renormalized energy site. We got rid of the bond energy β subscripts, which we have tagged with a superscripts z since it is pair-sugar bond energy (and later b for pair-pair bond energy), and we indistinguish the site energies, as we assume, they have the same magnitude.

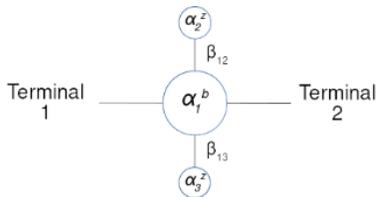


Figure 2. A base pair with its respective sugars connected to molecular terminals

The process is illustrated in Figure 3.

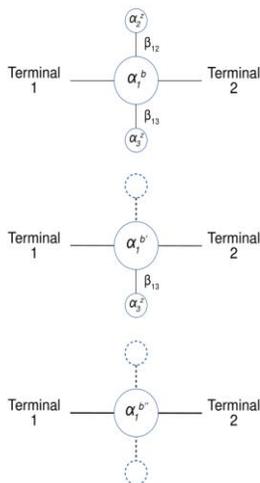


Figure 3. Renormalization procedure of a DNA base pair

Once obtained the renormalization equation, we may acquire the equations for an effective dimer that contains information of any numbers of base pairs; equations for a trimer and a dimer shall be

obtained, as seen in Figure 4.

Here, α_j are the respective energies given by (2) and $\chi_{ij} = \kappa_n \beta_{ij}^b$, with κ_n defined as a deformation coefficient. The latter will help us to parameterize changes in specific bonds that will later represent deformation in the system.

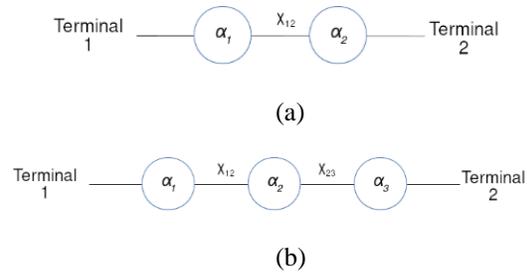


Figure 4. Wires of (a) two and (b) three base pairs, each site of the dimer (trimer) represents a base pair dimer *per se*.

Expanding (1) for the dimer we obtain:

$$\alpha_1 = \alpha_1 + \beta X_1^{-1} \quad (3)$$

$$\alpha_2 = \alpha_2 + \beta^2 \zeta_1^{-1} \quad (4)$$

$$\beta_{12} = \beta^b \kappa_1 \quad (5)$$

and for the trimer:

$$\alpha_1 = \alpha_1 + \beta^b \eta_1^2 X_1^{-1} (1 + \kappa_1^2 \zeta_3 X_1^{-1} \Gamma^{-1}) \quad (6)$$

$$\alpha_6 = \alpha_3 + \beta^b \eta_3^2 X_3^{-1} (1 + \kappa_2^2 \zeta_1 X_3^{-1} \Gamma^{-1}) \quad (7)$$

$$\beta_{16} = \beta \eta_1 \eta_2 \eta_3 (\kappa_1 \kappa_2) X_1^{-1} X_2^{-1} \Gamma^{-1} \quad (8)$$

where $X_n = (E - \alpha_n)/\beta$ is the dimensionless reduced energy [3], $\zeta_1 = X_2 - \kappa_1^2/X_1$, $\zeta_3 = X_2 - \kappa_2^2/X_3$ and $\eta_n = \beta_n/\beta$, but since we don't have different inter-base-base bond energies, then $\eta_n = 1$. It is clear to see that, if $\kappa_n = 1$, the results of [3] are recovered. With these equations we may build a cable constituted of any number of base pairs, substituting the sites and bond energies on themselves recursively.

2.2 Transmission coefficient



For calculating the transmission coefficient of the system, we used the Lippmann-Schwinger equation in its discrete form:

$$\psi(x) = \psi^0(x) + \sum_{l,m} G^0(n,l)V(l,m)\psi_m(x) \quad (9)$$

here, $\psi(x)$ and $\psi^0(x)$ are the perturbed and free wave function, respectively, $G^0(n,l)$ is the unperturbed Green function of the system, which for an atomic wire is [7]:

$$G^0(n,l) = \langle n|G^0|l \rangle = \frac{ie^{i|n-l|x}}{2\beta\sin(x)} \quad (10)$$

and V is the potential, which is the scattering potential for an electron propagating through the atomic wire with a dimer impurity (see Figure 5), that is:

$$V = 2\beta \gamma(|0\rangle\langle 0| + |0\rangle\langle 0|) \quad (11)$$

whence, β is the bond energy, $z_{0,1} = (\alpha_{0,1} - \alpha)/2\beta$ and $\gamma = (\beta_{01} - \beta)/2\beta$ are the reduced site and bond energy, respectively, and $|0\rangle, |1\rangle$ are the wave function states on those sites, as illustrated in figure 5.

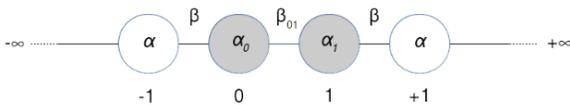


Figure 5. Scattering potential for an electron propagating through the atomic wire

For a free particle entering the system, equation (9) can be rewritten as:

$$\tau e^{ikx} = e^{ikx} + \sum_{l,m} \frac{ie^{i|n-l|x}}{2\beta\sin(x)} V(l,m)\psi_m(x) \quad (12)$$

with τ being the transmission coefficient. Solving (12) for the transmittance $T = |\tau|^2$ yields:

$$T = \frac{(1+2\gamma)^2(4-X^2)}{(1-2Q)^2(4-X^2)+4(P-QX)^2} \quad (13)$$

where

$$P = z_0 + z_1 \quad (14)$$

$$Q = z_0z_1 - \gamma - \gamma^2 \quad (15)$$

With (13) we can obtain the $T(E)$ profiles. For that, we may set the particular dimensionless values for the atomic sites of $\alpha_b = \alpha_z = 0$, the bond energies $\beta = -0.25$ and $\beta^{(z)} = 2\beta = -0.5$, this being noted in experiments: base-sugar bond energy doubles base-base bond energy [4], and a bandwidth of $E = [-4\beta, 4\beta]$.

2.3 Current through the system

The current I can be calculated with [8]:

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E)[f_L(E) - f_R(E)]dE \quad (16)$$

Here, $T(E)$ is the Transmission-Energy profile for a 30-base pair DNA wire, $f_{L/R}(E) = \{exp$ is the Fermi function, h and e are the Planck constant and the electron charge, respectively. The room temperature is set $k_B T = 26meV$ to make resemblance with the experiment [4]. μ_L and μ_R are the electrochemical potentials of the electrodes, given by [8] $\mu_L = E_f + (1+k)eV$ and $\mu_R = E_f - keV$, where E_f and V are the equilibrium Fermi energy and the applied voltage, respectively. The parameter k describes how the applied voltage is divided across the electrodes and the molecule. We then set the parameters of the system to real experimental values [5]: $\beta = -0.37eV$, $\beta^{(z)} = -0.74eV$, $\alpha_b = \alpha_z = 0$, a fixed Fermi energy $E_f = 2.12eV$, and $k = 2/5$ instead of $1/2$ or $1/3$ of other works [1].

3. Results

In figure 6 and 7 are presented the $T(E)$ profiles of 2,3,4 and 10 base pair chains.

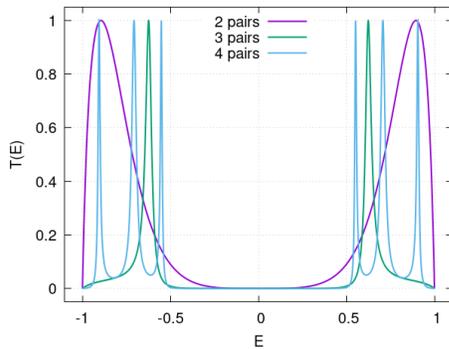


Figure 6. Transmission through 2, 3 and 4 base pairs

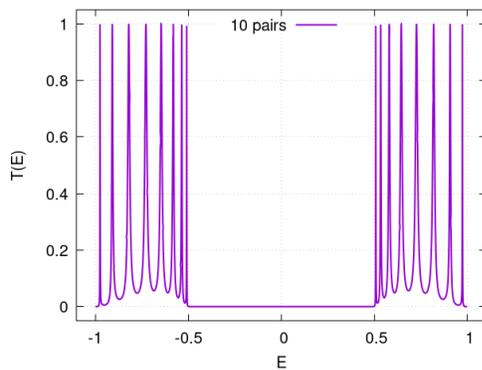
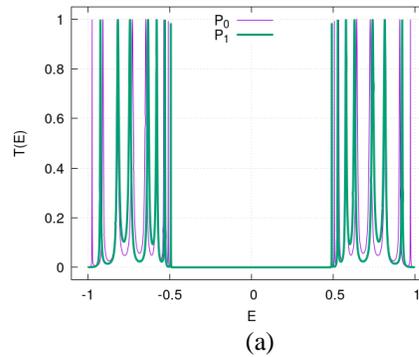
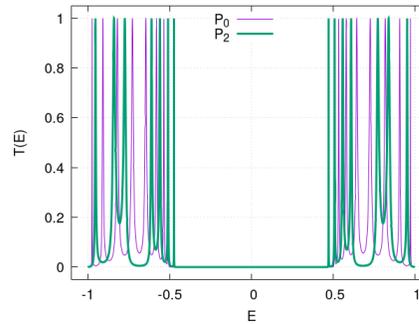


Figure 7. Transmission through 10 base pairs

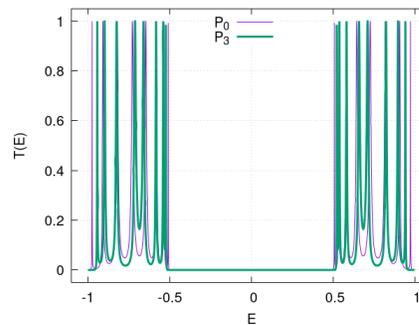
We see from the former a well-defined gap for energies between -0.5 and 0.5 where transport does not occur, and resonances ($T = 1$) depending on the number of base pairs in the chain. This is important since it can be interpreted as a semiconductor, where a minimum of energy shall be applied for conduction to take place. Figure 8 shows different 10 base pairs $T(E)$ plots where deformation profiles are applied, being: P_0 is unperturbed, $P_1: \kappa_1 = 1, \kappa_2 = 1.25, \kappa_3 = 1.25, \kappa_4 = 1$, and $P_2: \kappa_1 = 1.25, \kappa_2 = 1.5, \kappa_3 = 1.5, \kappa_4 = 1.25$, representing an increment on the central part of the wire; $P_3: \kappa_1 = 1, \kappa_2 = 0.75, \kappa_3 = 0.75, \kappa_4 = 1$ and $P_4: \kappa_1 = 0.75, \kappa_2 = 0.5, \kappa_3 = 0.5, \kappa_4 = 0.75$, representing a decrement on the central part of the wire. We see that gaps are generated between resonances, at low energies for the profiles P_1 and P_2 , and at higher for P_3 and P_4 .



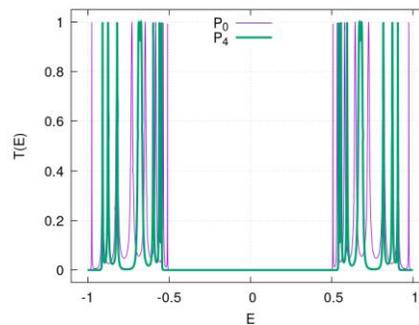
(a)



(b)



(c)



(d)

Figure 8. Transmission onto the deformation profile (a) P_1 , (b) P_2 , (c) P_3 , (d) P_4 in comparison with P_0 .

Figure 9 shows the $I - V$ curve for the theoretical result of (16) in comparison with the experimental data of Porath *et al* [4].

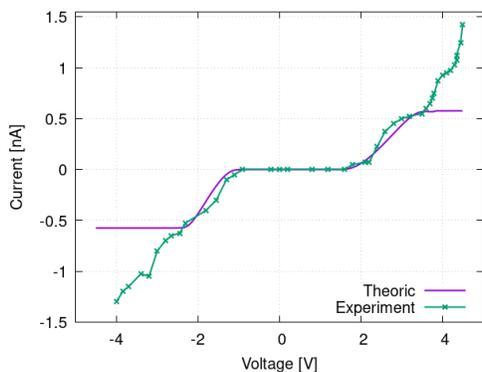


Figure 9. Current through a 30-base pair wire

The proposed model makes a well approximation within the gap interval, and then it saturates at high voltages. Saturation might be given by the short bandwidth utilized for first neighbors.

4. Conclusions

We see that, for each added base pair resonances appear, and the gap is more defined. These results allow us to infer that, given a deformation on the system, there will be intervals where transmittance keeps its maximum value. These intervals are optimal for building molecular wires that, although deformed, can transport a desirable amount of charge. Also, where a gap will be generated, whose application may be as molecular sensors that can detect a resonance shift. The $I - V$ curve makes a good resemblance with the experimental data. This shows the effectiveness of the model besides the simplification taken. Future work involves sequence engineering for building wires with different nitrogenous bases, exploring decoherence within the system and tight binding

for second neighbors.

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