

## Influence of solitons on the conductance properties of double-stranded deoxyribonucleic acid

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**Abstract.** A numerical study is presented to investigate the role of solitons in the electronic states of double-stranded DNA (dsDNA) molecule in the metal/DNA/metal system. Based on tight-binding Hamiltonian model and within the framework of a generalized Green's function technique, we consider a ladder model for poly(dG)-poly(dC) DNA molecule containing  $M$  cells with four sites (two base pair sites and two backbone sites) in each cell. In the presence of a sublattice of solitons, our results show that the homogeneous soliton distributions induce the electronic states in the band gap of DNA molecule. In addition, the room temperature current–voltage characteristic of the system shows a linear and ohmic-like behaviour.

**Keywords.** Deoxyribonucleic acid; electronic transmission; soliton; ladder model; Green's function.

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### 1. Introduction

During the last few years, many studies have been devoted to understand the conduction properties of electrode–(single)molecule–electrode systems in the framework of molecular electronics [1–7]. Single molecules with semiconducting behaviour play an important role in the development of these systems for electronic applications. The discovery that deoxyribonucleic acid (DNA) can conduct electrical current has made it an interesting candidate for the roles that nature did not intend for this molecule. In particular, DNA could be useful in nanoelectronics for designing electric circuits, which could help to overcome the limitations that silicon-based electronics is facing in recent years. However, DNA electronics does not aim to make something new. Its immediate goal is to improve old concepts in a new manner, although in the process it may create entirely new ideas in nanoelectronics [8–10]. Many experimental groups have reported measurements of the

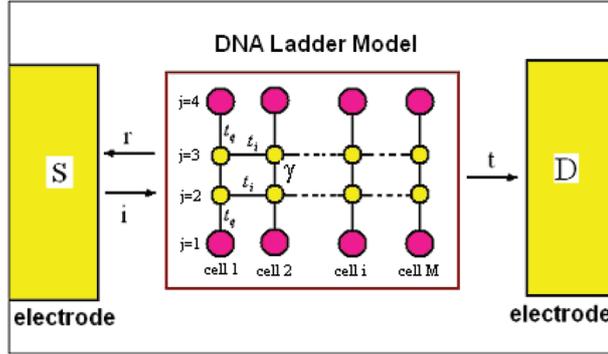
current–voltage characteristics of DNA molecules which are, however, quite controversial [11,12]. It has been found that the observed conductance of DNA molecule varies from insulating to metallic behaviour [13–16]. In particular, the Porath *et al* experiments [17] based on which, DNA molecule as a poly(dG)–poly(dC) sequence has electrical characteristics similar to that of a semiconductor diode, that allow current to flow in just one direction, have stimulated some research interest in the transport properties of DNA. Accordingly, DNA may be an excellent candidate for molecular electronics and may serve as a molecular wire, transistor, switch or rectifier depending on its electronic properties [11,18].

The double-stranded DNA structure undergoes a very complex dynamics and the knowledge of this dynamics provides a deeper understanding of the electronic and structural properties of DNA molecule. The possibility that the existence of nonlinear excitations, such as solitons, may affect the functional properties of DNA, has been the topic of intensive research [19–24]. In this paper, we study the effects of solitons, which are induced via nonlinear potential representing the hydrogen bonds between guanine (G) and cytosine (C) bases, on the electronic conduction properties of poly(dG)–poly(dC) DNA in metal/DNA/metal system. According to our model, in the presence of a sublattice of solitons, the band gap of the semiconductor structure of DNA molecule may be suppressed and at room temperature, it's current–voltage characteristic shows an ohmic-like behaviour. In our model, a ladder model is considered for DNA molecule consisting of G and C strands which, coupled by nonlinear hydrogen bonds, are sandwiched between two semi-infinite metallic leads as electrode (electron reservoirs). The model and a description of the computational methods for investigating the conductance properties of the model structure are introduced in §2. The results and discussion are presented in §3, followed by conclusion in §4.

## **2. Model and methodology**

As it is well-known, the nature of charge transfer and electron transport through DNA molecule depends on the understanding of its structural parameters. DNA consists of a double-helix with an aromatic  $\pi$ -stack core where four types of nucleobase participate in Watson–Crick base pairing [25]. A detailed understanding of DNA structure suggests that the  $\pi$ – $\pi$  interaction between the stacked base pairs in DNA could support extended charge transport. The double-stranded DNA could offer pathways for long-range charge transport. The electronic coupling through a duplex stack of nucleobases is expected to involve both intrastrand and interstrand pathways [26].

Here we consider a model for DNA molecule which exhibits a semiconducting gap clearly and includes the backbone structure of DNA explicitly. DNA molecule in poly(dG)–poly(dC) ladder model has two central conduction channels in which the base pairs are interconnected and further linked to upper and lower sites, representing the backbone. The backbone sites, however, are not interconnected along the DNA sequence [18]. In our model the DNA structure with  $M$  cells with four sites in each cell is set between two semi-infinite metallic leads as the electrodes and then the conductance properties of the system are numerically investigated based on



**Figure 1.** The schematic representation of the dsDNA molecule model sandwiched between two semi-infinite metallic electrodes. Pink (yellow) circles represent the backbone (base) sites.

the well-known procedures particularly suitable to treat the electron transmission through the mesoscopic structures, Landauer formalism and a generalized Green's function method. As illustrated in figure 1, each cell connects to the left (right) cell through two horizontal hopping integrals,  $t_i$ . Also in a typical cell the base pair sites connect to each other through hopping integral  $\gamma$  and connect to upper and lower backbone sites via vertical hopping integrals,  $t_q$ . In addition, the first (end) cell, via the linker groups, may be connected to left (right) leads as the electron reservoirs. In this study we consider a ladder model for DNA molecule containing  $M = 64$  cells.

We use the following generalized Hamiltonian for the description of the metal/DNA/metal structure:

$$H = H_m + H_{\text{DNA}} + H_c, \quad (1)$$

where  $H_m$ ,  $H_{\text{DNA}}$  and  $H_c$  describe the semi-infinite metallic contacts, the DNA Hamiltonian and the couplings of the contacts to DNA molecule, respectively. The metallic electrodes (electron reservoirs) are modelled within the tight-binding approximation with only one electron per site. Accordingly,  $H_m$  can describe reasonably well the band structure of a one-dimensional chain especially near the Fermi level which is considered zero in this case since the on-site energy is assumed to be zero,

$$H_m = \sum_i \varepsilon_i |i\rangle \langle i| - \sum_i t_{i,i+1} |i\rangle \langle i+1| + \text{h.c.}, \quad (2)$$

where  $|i\rangle$  denotes the electron state in the reservoirs. For the semi-infinite metallic contacts we set  $\varepsilon_i = \varepsilon_0$  for all  $i$  and  $t_{i,i\pm 1} = t_0$  between all  $i$  and  $i \pm 1$  for the nearest-neighbour hopping. With  $\varepsilon_i = 0$  we have set the zero of energy at the Fermi level.  $H_c$  denotes the interacting Hamiltonian between DNA molecule and metallic contacts and is given as

$$H_c = -t_c (|i\rangle \langle 1| + |M\rangle \langle i|). \quad (3)$$

Here  $t_c$  denotes the interaction strength between single electron states of base-pairs in the cell of number 1(M) from the left (right) of DNA molecule and the electron states in the left (right) electrode. Using the Löwdin's matrix partition technique [27], we may rewrite the Hamiltonian of the total system as follows:

$$H_{\text{eff}} = -\Sigma^L|1\rangle\langle 1| + H_{\text{DNA}} - \Sigma^R|M\rangle\langle M|, \quad (4)$$

where  $\Sigma^L(\Sigma^R)$  is the self-energy matrix resulting from the coupling of the DNA molecule to the left (right) electrode. Now considering the ladder model for DNA molecule, according to figure 1, the effective Hamiltonian (4) can be expressed in matrix form as follows:

$$H_{\text{eff}} = \begin{bmatrix} \mathbf{H}_1 & \mathbf{T}_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ \mathbf{T}_1^+ & \mathbf{H}_2 & \mathbf{T}_2 & 0 & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \mathbf{T}_2^+ & \mathbf{H}_3 & \ddots & 0 & \vdots & \vdots & \vdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 & \vdots & \vdots & \vdots \\ \vdots & \vdots & 0 & \ddots & \mathbf{H}_{i-1} & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & \mathbf{T}_{i-1}^+ & \mathbf{H}_i & \mathbf{T}_i & 0 & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \mathbf{H}_{i+1} & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \mathbf{T}_{M-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \mathbf{T}_{M-1}^+ & \mathbf{H}_M \end{bmatrix}, \quad (5)$$

where  $\mathbf{H}_i$  is a  $4 \times 4$  three-diagonal matrix describing the four sites within the  $i$ th cell (figure 1) and  $\mathbf{T}_{i-1}^+$  and  $\mathbf{T}_i$  are  $4 \times 4$  matrices describing the hopping to and from cell  $i$ . Thus

$$\begin{aligned} \mathbf{H}_1 &= \begin{bmatrix} \varepsilon_{11} & t_q & 0 & 0 \\ t_q & \varepsilon_{12} - \Sigma_{12} & \gamma & 0 \\ 0 & \gamma & \varepsilon_{13} & t_q \\ 0 & 0 & t_q & \varepsilon_{14} \end{bmatrix}; \\ \mathbf{H}_M &= \begin{bmatrix} \varepsilon_{M1} & t_q & 0 & 0 \\ t_q & \varepsilon_{M2} & \gamma & 0 \\ 0 & \gamma & \varepsilon_{M3} - \Sigma_{M3} & t_q \\ 0 & 0 & t_q & \varepsilon_{M4} \end{bmatrix}, \\ \mathbf{H}_i &= \begin{bmatrix} \varepsilon_{i1} & t_q & 0 & 0 \\ t_q & \varepsilon_{i2} & \gamma & 0 \\ 0 & \gamma & \varepsilon_{i3} & t_q \\ 0 & 0 & t_q & \varepsilon_{i4} \end{bmatrix}; \quad 1 < i < M; \\ \mathbf{T}_i &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & t_i & 0 & 0 \\ 0 & 0 & t_i & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \end{aligned} \quad (6)$$

where  $\varepsilon_{ij}$  with  $i = 1, \dots, M$  and  $j = 1, 2, 3, 4$  are the on-site energies within each cell, which are considered to be zero. Also  $z = E + i0^+$  is considered to be a

complex number whose real part,  $E$  is the energy at which the transfer occurs. In addition, in cell 1(M) with  $j=2(3)$ ,  $\Sigma_{ij} = \Sigma$  is considered. Using Dyson equation, the self-energy  $\Sigma$  may be carried out as [28]

$$\Sigma = \frac{t_c^2}{E - \varepsilon_0 - \Gamma}, \quad (7)$$

where  $\Gamma$  is the self-energy correction of the metallic contacts to the ending-sites attached to the DNA molecule, and has the following expression [29]:

$$\Gamma = \left( \frac{E - \varepsilon_0}{2} \right) - i \left[ t_0^2 - \left( \frac{E - \varepsilon_0}{2} \right)^2 \right]^{1/2}. \quad (8)$$

Here  $\varepsilon_0 = 0$  and  $t_0 = 1$  eV are the on-site energy and the nearest-neighbour hopping integral of the metallic contacts, respectively. The semiconducting behaviour of the dsDNA molecule may be explained by the measured room temperature  $I$ - $V$  characteristic with a band gap of the order of 1 eV [8,17]. This semiconducting feature may be controlled via the modification of the coupling strength between G and C bases which is given as

$$\gamma_{n,n+1} = \gamma_0 + \alpha(u_n - u_{n+1}), \quad (9)$$

where  $n$  runs over the site index of the bases.  $\alpha = 2.8(\alpha_0\gamma_0)\sin^2(\theta_0/2)$  and  $u_n$  are the electron-twist coupling parameter [30,31] and the displacement of  $n$ th base on each strand, respectively. The quantity  $\alpha_0 = 0.383333 \text{ \AA}^{-1}$  regulates how strong  $\gamma_{n,n+1}$  is influenced by  $u_n$ . Also  $\gamma_0 = 0.037$  eV is the equilibrium value of the hopping integral between G and C bases and  $\theta_0 = 36^\circ$  is the equilibrium twist angle between two consecutive base pairs [31]. In dsDNA, solitons (geometrical defects) correspond to the phonon field configurations resulting from the displacement of bases on each strand leading to a change in the equilibrium length of the hydrogen bonds and may effectively influence the electronic conduction through DNA. In the presence of solitons, the displacement of a base on each strand is determined in such a way as to give optimum shape for the soliton. Accordingly, the displacements of bases from their equilibrium positions in the  $n$ th cell are modelled as [21,23]

$$u_n = u_0 \prod_m \operatorname{sech} \left[ \frac{(n-m)a}{\xi} \right]. \quad (10)$$

Here  $a = 3.4 \text{ \AA}$  is the distance between two consecutive base pairs (cells) along the molecule,  $2\xi = 16a$  is the width of a soliton and  $ma$  is the location of the  $m$ th soliton centre on each strand. In addition,  $u_0$  is considered to be the maximum amplitude of a soliton at the half-width. Here  $u_0 = 14.25 \text{ \AA}$  is set.

Now we proceed to determine the conductance of the metal/DNA/metal structure. The most commonly used computational schemes for calculating the (coherent) conductance  $g$  are the Landauer theory [32] and the Green's function formalism [33,34]. The conductance  $g$  is simply proportional to the transmission coefficient,  $T(E)$ , for injected electrons at the Fermi energy:

$$g = g_0 T(E); \quad g_0 = \frac{2e^2}{h}. \quad (11)$$

The transmission coefficient can be calculated from the knowledge of the molecular energy levels, the nature and the geometry of the contacts. To connect the Green's function with the transmission coefficient between reservoirs we consider a linear transport between them. Using the Fisher–Lee formalism [35] the differential conductance may be expressed as

$$g = g_0 |G_{1M}(E)|^2 \Delta_1(E + eV) \Delta_M(E), \quad (12)$$

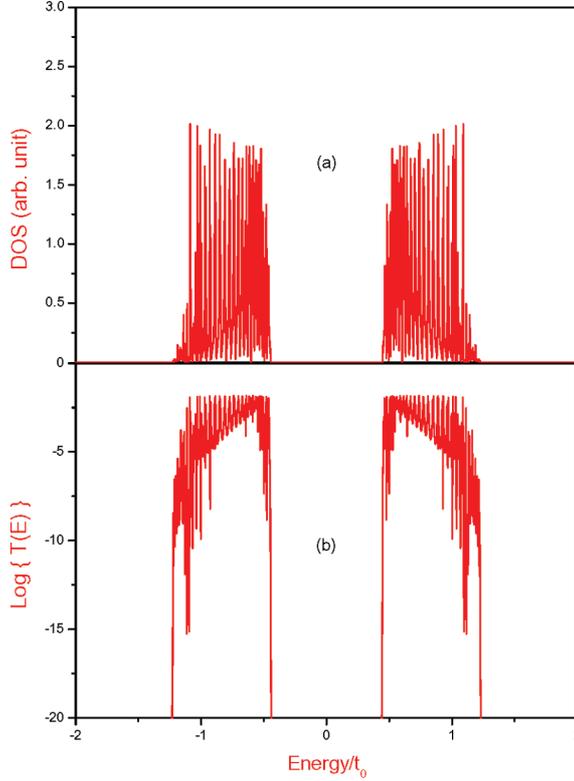
where  $G_{1M}(E)$  is the matrix element of  $G(E) = (E - H_{\text{eff}})^{-1}$  between the molecular sites in the 1 and M cells connecting the left and right reservoirs, respectively. To calculate  $G_{1M}(E)$ , we have generalized the procedures suggested in refs [36–38] to our model for dsDNA in the metal/DNA/metal system. To simplify the calculations,  $\Delta_1 (= \Delta_M) = \Delta$  is considered.  $\Delta = \text{Im}\{\Sigma\}$  is the chemisorption coupling at the metal/molecule interface. The effect of the metallic electrodes may be lumped into the energy of the molecular sites that are coupled to the electrodes. In our model the energies of these sites are described via the matrix elements of  $(H_1)_{22}$  and  $(H_M)_{33}$  in eq. (6).

### 3. Results and discussion

Based on the formalism described in §2, we have investigated some of the significant properties of electronic conduction of metal/DNA/metal system. To proceed, first we study the electronic density of states (DOS) and the electron transmission coefficient,  $T(E)$ , through dsDNA molecule in the foregoing structure. In the absence of solitons, panels (a) and (b) in figure 2 illustrate the DOS and the logarithm of  $T(E)$  for the metal/DNA/metal structure, respectively. DNA molecule has  $N = 64$  base pairs (bps). Here the metal/molecule coupling strength and the hopping integral in the metallic contacts are set as  $t_c = 0.3$  eV and  $t_0 = 1$  eV, respectively. Figure 2 displays the semiconducting behaviour of DNA molecule in the model with  $\approx 0.95$  eV energy gap, clearly.

Our calculations show that the existence of solitons markedly affects the electronic structure of dsDNA and gives rise to the modification in semiconducting behaviour of DNA molecule. The presence of solitons induces electronic states within the band gap and causes an enhancement in the conductance of the metal/DNA/metal system. Using model parameters as in figure 2, panels (a) and (b) in figure 3 illustrate the DOS and the logarithm of  $T(E)$ , in the presence of solitons, for the metal/DNA/metal structure, respectively. As clearly seen, the band gap has filled and due to the increasing overlap between electronic states, the conductance of the system has been increased.

The current–voltage ( $I$ – $V$ ) characteristic of the system is investigated in figure 4. In order to calculate the current through metal/DNA/metal structure, we consider the standard transport formalism of electric current under an applied potential bias of  $V$  [26,39],



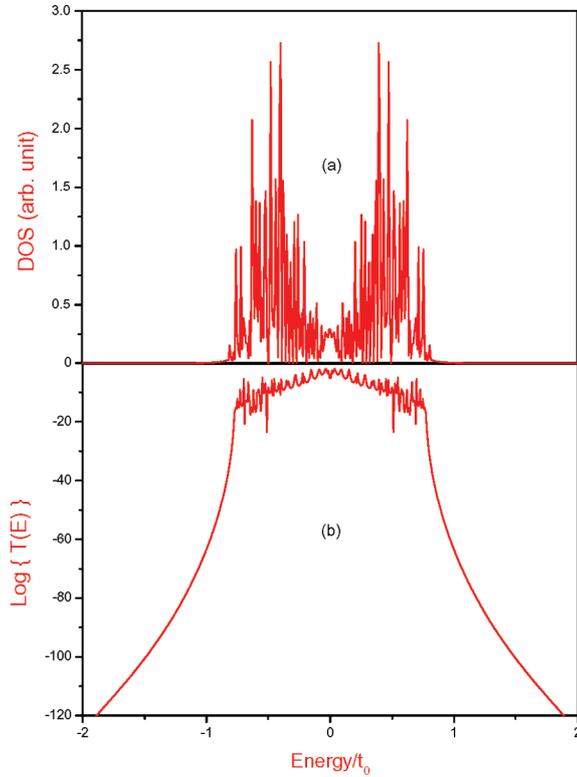
**Figure 2.** Panels (a) and (b) show the electronic density of states (DOS) and the logarithm of the transmission coefficient vs. the dimensionless parameter  $\text{Energy}/t_0$  for the metal/DNA/metal system in the absence of solitons. Using the model parameters as mentioned in the text, we set  $t_0 = 1$  eV,  $t_c = 0.3$  eV,  $t_i = 0.37$  eV,  $t_q = 0.74$  eV,  $\gamma_0 = 0.037$  eV and 64 bps for DNA molecule.

$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} dE T(E) W(E - E_F; eV), \quad (13)$$

where  $T(E)$  denotes the electron transmission coefficient of DNA molecule in the metal/DNA/metal structure and  $E_F$  is the Fermi energy of the metallic electrodes,

$$W(E, eV) = f(E) - f(E + eV), \quad (14)$$

with the Fermi function  $f(E) = (e^{\beta E} + 1)^{-1}$  and  $\beta = t/(k_B T)^{-1}$ . The Fermi function is the difference between charge distributions before and after transport [39,40]. The driving force here is the electric potential bias. Figure 4 shows the room temperature  $I$ - $V$  characteristics of the system in the absence (dashed curve) and in the presence (solid curve) of solitons in dsDNA structure. The dashed curve shows clearly a nonlinear dependence. Our results show a good qualitative agreement with the energy gap of DNA along the zero current part of the  $I$ - $V$  curve in the absence of solitons. In other words, the low-voltage part of the dashed  $I$ - $V$  curve



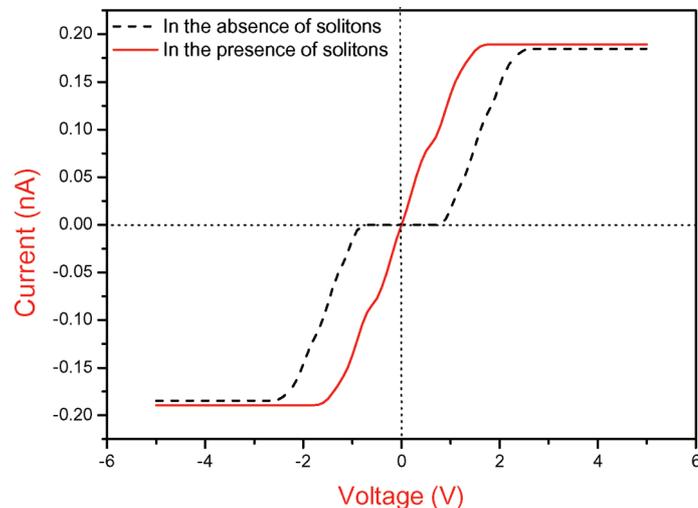
**Figure 3.** Panels (a) and (b) show the electronic density of states (DOS) and the logarithm of the transmission coefficient vs. the dimensionless parameter  $Energy/t_0$  for the metal/DNA/metal system in the presence of solitons. The model parameters used are as mentioned in figure 2.

arises from the semiconducting behaviour of poly(dG)–poly(dC) DNA molecule. On the other side, the presence of solitons in dsDNA structure crucially modifies this behaviour (solid curve) and the  $I$ – $V$  characteristic of the system shows a linear and ohmic-like behaviour.

#### 4. Conclusion

To conclude, based on the presented methodology and our model in §2, we have investigated the effect of the presence of solitons on the electronic conduction properties of poly(dG)–poly(dC) DNA molecule in the metal/DNA/metal system. Considering dsDNA molecule as a ladder model, our results suggest that the semiconducting behaviour of DNA may be modified due to the existence of solitons, which are induced via nonlinear potential representing the hydrogen bonds between guanine (G) and cytosine (C) bases, so that in the presence of a sublattice of solitons, the band gap of the semiconductor structure of DNA molecule is suppressed and

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**Figure 4.** The current–voltage characteristics of DNA molecule at room temperature ( $T = 300$  K) in the absence (dashed curve) and in the presence (solid curve) of solitons for the metal/DNA/metal system. The model parameters used are as mentioned in figure 2.

the room temperature  $I$ – $V$  characterization of the molecule shows an ohmic-like behaviour.

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