Transport properties of poly(GACT)–poly(CTGA) deoxyribonucleic acid: A ladder model approach

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Abstract. In this paper, based on the tight-binding Hamiltonian model and within the framework of a generalized Green's function technique, the electronic conduction through the poly(GACT)–poly(CTGA) DNA molecule in SWNT/DNA/SWNT structure has been numerically investigated. In a ladder model, we consider DNA as a planar molecule containing M cells and four further sites (two base pair sites and two backbone sites) in each cell, sandwiched between two semi-infinite single-walled carbon nanotubes (SWNT) as the electrodes. Having relied on Landauer formalism, we focussed on studying the current–voltage characteristics of DNA, the effect of the coupling strength of SWNT/DNA interface and the role of tube radius of nanotube contacts on the electronic transmission through the foregoing structure. Finally, a characteristic time was calculated for the electron transmission, which measures the delay caused by the tunnelling through the SWNT/DNA interface. The results clearly show that the calculated characteristic time and also the conductance of the system are sensitive to the coupling strength between DNA molecule and nanotube contacts.

1. Introduction

The discovery that the deoxyribonucleic acid (DNA) can conduct the electric current, has made it an interesting candidate for the roles that nature did not intend for this molecule. In particular, the DNA could be useful in nanoelectronics for designing the electric circuits, which could help to overcome the limitations that silicon-based electronics is facing in recent years. However, the DNA electronics does not aim to make something new. Its immediate goal is to improve the old concepts in a new manner, although it may create entirely new ideas in nanoelectronics during the process [1–3]. The nanoelectronic devices have been usually designed in such a way that a single molecule is sandwiched between two electrodes (metallic or organic). Considering the immense progresses in the field of nanofabrication, studies have been undertaken towards the structures, such as carbon nanotubes

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(CNTs), as the nanoelectrodes [4–7]. The significantly improved switching characteristics of the short organic field effect transistors (FET) with CNT electrodes compared to the metallic ones are attributed to the excellent electrostatics attainable with the nanotube electrode geometry [8,9]. A number of experimental groups have reported the measurements of the current–voltage characteristics of the DNA molecule, which are, however, still quite controversial [10,11]. The DNA may be an insulator [12,13], a semiconductor [14] or a metal [15,16]. In particular, the Porath *et al* experiments [14], based on which, the DNA molecule is considered as a 10.4 nm long sequence, has an electrical characteristics similar to those of semiconductor diodes, which allows the current to flow in just one direction have stimulated some research interests towards the transport properties of the DNA. Accordingly, the DNA may be an excellent candidate for the molecular electronics and may serve as a molecular wire, transistor, switch or rectifier depending on its electronic properties [10,17]. Also, several theoretical models, which range from the quantum mechanical approaches, mostly use strictly one-dimensional tight-binding models [18–21] to the density functional theory [22], have been developed for investigating the electron transport properties of the DNA molecule. Several studies on the structural, electronic and conduction properties of the DNA have been published [15–20]. Most studies have been focussed on understanding the details of the DNA electronic structures, the nature of electronic states, impurities and how the geometrical factors affect the conduction properties of the DNA in the nanoelectronics devices [1–4,23]. However, there are some significant factors, the influences of which on the conductance through the electrode–(single)molecule–electrode structure have not yet been fully studied. For example, the role of the radius of nanotube electrodes [24] and the contact-dependent effects on the electronic transmission through the molecule [25] and also the issue of how long the tunnelling electron actually spends through the electrode/molecule interface potential are of particular interest [26,27]. Here, we focus on the role of SWNT/DNA coupling strength, as an important parameter in studying the electronic transport through the DNA. We calculate an interaction time for the electron tunnelling through the SWNT/DNA interface. It is shown that there is a close relationship between the coupling strength in the interface and the above time-scale. We find that, as the coupling strength between the CNT electrodes and the DNA molecule increases, the tunnelling time sharply decreases. In the presented model, the typical system is considered as a planar DNA molecule sandwiched between two semi-infinite armchair (l, l) single-walled carbon nanotubes (SWNT) as the nanoelectrodes (figure 1). The model and the explanation of the computational methods for the study of the conductance properties of the model structure are introduced in §2. The results and discussion are presented in §3, followed by the conclusion in §4.

2. Methodology

As it is well-known, the nature of charge transfer and electron transport through the DNA molecule depends on the understanding of its structural parameters. The DNA consists of a double-helix with an aromatic π-stack core, where four types of nucleobases (thymine, T; cytosine, C; adenine, A; guanine, G) participate in
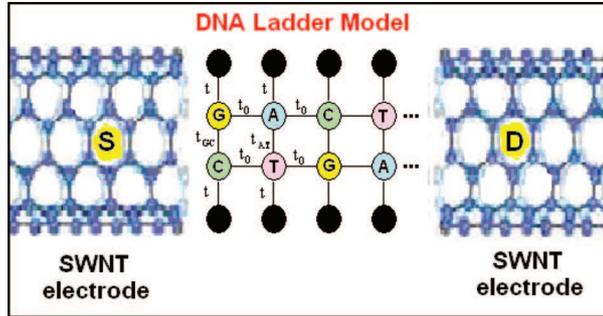
Figure 1. A schematic representation of the SWNT/DNA/SWNT structure. The suggested ladder model for the DNA contains the cells connecting each other.

Watson–Crick base pairing (G:C; A:T) [28]. A detailed knowledge of the DNA structure suggests that the π–π interaction between the stacked base pairs in the DNA could support extended charge transport. The density-functional calculations [22] have shown that the bases, especially guanine, are rich in π-orbitals. The double-strand DNA could offer pathways for the long-range charge transport. The electronic coupling through a duplex stack of nucleobases is expected to involve in both intrastrand and interstrand pathways [29]. Here, we consider a ladder model to study the DNA electronic properties, which includes the backbone structure of the DNA, explicitly. As shown in figure 1, the DNA molecule in the ladder model have two central conduction channels in which G and C (A and T) sites represent a base-pair (bp), which are interconnected and further linked to the upper and lower sites, representing the backbone. The backbone sites, however, are not interconnected along the DNA sequence [17]. In the presented model, the DNA structure as a two-dimensional layer, consisting of M cells and further four sites in each cell, is set between two semi-infinite armchair (n,n) SWNTs as the electrode and then the conductance properties of the system is numerically calculated, based on well-known procedures particularly suitable for treating 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_0. Also, in a typical cell, the base-pair sites connect to each other through a hopping integral $t_{\mathrm{GC}}(t_{\mathrm{AT}})$ and connect to the upper and lower backbone sites via vertical hopping integrals, t. The first(end) cell, via the linker groups, may be connected to the left(right) semi-infinite armchair (l, l) SWNT as a nanocontact. In this study, we consider a ladder model for the DNA molecule of $M = 32$ cells (128 sites), in which the nanocontacts are considered to be the armchair (5,5).

2.1 *The Hamiltonian model*

The following generalized Hamiltonian is considered for the description of the SWNT/DNA/SWNT structure:

$$H = H_{\text{SWNT}} + H_{\text{DNA}} + H_{\text{C}}, \tag{1}$$

where H_{SWNT}, H_{DNA} and H_{C} describe the semi-infinite SWNT nanocontacts, the DNA Hamiltonian and the couplings of the contacts to DNA molecule, respectively. The SWNTs (electron reservoirs) are modelled within the tight-binding approximation with only one π-orbital per atom. Accordingly, H_{SWNT}, which can describe well reasonably the band structure of a nanotube, especially near the Fermi level, which is considered zero in this case, because the on-site energy is assumed to be zero and each orbital is half-filled,

$$H_{\text{SWNT}} = \sum_i \varepsilon_i |i\rangle\langle i| - \sum_i t_{i,i+1} |i\rangle\langle i+1| + \text{h.c.}, \tag{2}$$

where $|i\rangle$ denotes the electron state in the reservoirs. For the semi-infinite SWNT contacts, we set $\varepsilon_i = \varepsilon_0$ for all i and also $t_{i,i\pm1} = t_{\text{SWNT}}$ between all i and $i \pm 1$ for the nearest-neighbour hopping. H_{C}, which denotes the interacting Hamiltonian between the DNA molecule and the nanotube contacts, is given as

$$H_{\text{C}} = -t_c(|i\rangle\langle 1| + |M\rangle\langle i|). \tag{3}$$

Here, t_c denotes the interaction strength between the single electron states of base-pairs in the cell of number $1(M)$ from the left(right) and the electron states in the left(right) electrode of the DNA molecule. Using the Löwdin's matrix partition technique [30], we may rewrite the Hamiltonian of the total system as follows:

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

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

$$H_{\text{eff}} = \begin{bmatrix} H_1 & T_1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ T_1^+ & H_2 & T_2 & 0 & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & T_2^+ & H_3 & \ddots & 0 & \vdots & \vdots & \vdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 & \vdots & \vdots & \vdots \\ \vdots & \vdots & 0 & \ddots & H_{i-1} & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & T_{i-1}^+ & H_i & T_i & 0 & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 & \ddots & H_{i+1} & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & T_{M-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & T_{M-1}^+ & H_M \end{bmatrix}, \tag{5}$$

where H_i is a 4×4 three-diagonal matrix describing the four sites within the ith cell (see figure 1) and T_{i-1}^+ and T_i are 4×4 matrices describing the hopping to and from the cell i. Thus:

Table 1. The rescaled tight-binding parameters used in this study [31].

On-site energies	Hopping integrals (eV)
$\varepsilon_{\mathrm{G}} = 0.633$	$t_{\mathrm{GC}} = 0.90$
$\varepsilon_{\mathrm{C}} = 0.723$	$t_{AT} = 0.34$
$\varepsilon_{\mathrm{A}} = 0.672$	$t = 1.50$
$\varepsilon_{\mathrm{T}} = 0.744$	$t_0 = 0.15$

$$
H_1 = \begin{bmatrix} \varepsilon_{11} & t & 0 & 0 \\ t & \varepsilon_{12} - \Sigma_{12} & t_{\mathrm{GC}} & 0 \\ 0 & t_{\mathrm{GC}} & \varepsilon_{13} - \Sigma_{13} & t \\ 0 & 0 & t & \varepsilon_{14} \end{bmatrix};
$$

$$
H_M = \begin{bmatrix} \varepsilon_{M1} & t & 0 & 0 \\ t & \varepsilon_{M2} - \Sigma_{M2} & t_{\mathrm{TA}} & 0 \\ 0 & t_{\mathrm{TA}} & \varepsilon_{M3} - \Sigma_{M3} & t \\ 0 & 0 & t & \varepsilon_{M4} \end{bmatrix}
$$

$$
H_i = \begin{bmatrix} \varepsilon_{i1} & t & 0 & 0 \\ t & \varepsilon_{i2} & t_{\mathrm{AT(CG)}} & 0 \\ 0 & t_{\mathrm{AT(CG)}} & \varepsilon_{i3} & t \\ 0 & 0 & t & \varepsilon_{i4} \end{bmatrix}; \quad 1 < i < M;
$$

$$
T_i = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -t_0 & 0 & 0 \\ 0 & 0 & -t_0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{6}
$$

Here, $i = 1$, M, $j = 2, 3$ and $\Sigma_{ij} = \Sigma$. The matrix of self-energies is defined as

$$
\Sigma^{\mathrm{L}} = \Sigma^{\mathrm{R}} = \Sigma_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Sigma & 0 & 0 \\ 0 & 0 & \Sigma & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{7}
$$

Also, $E_{ij} = \varepsilon_{ij} - z$ ($i = 1, \ldots, M$ and $j = 1, 2, 3, 4$), where ε_{ij} are the on-site energies within each cell, which is defined according to table 1 and $z = E + i0^+$ is the complex number whose real part, E, is the energy at which the transfer occurs. Here, the rescaled parameters are used for the on-site energies of poly(GACT)–poly(CTGA) structure, as listed in table 1. The parameters adapted for the effective Hamiltonian in this work are rescaled by $\varepsilon_{\mathrm{backbone}} = 12.27$ eV [31]. So, $\varepsilon_x = \varepsilon_x^0 / \varepsilon_{\mathrm{backbone}}$ with $x = $ G, C, A and T.

Now, the conductance of the SWNT/DNA/SWNT structure can be calculated, based on the above-suggested model Hamiltonian. The most commonly used computational scheme 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 the injected electrons at the Fermi energy:

$$g = g_0 T(E); \quad g_0 = \frac{2e^2}{h}. \tag{8}$$

The transmission coefficient can be calculated from the knowledge of the molecular energy levels, the nature and the geometry of the contacts. Using the Fisher–Lee formalism [35], the differential conductance may be expressed as

$$g = g_0 \left| G_{1M}(E) \right|^2 \Delta_1(E + eV)\Delta_M(E), \tag{9}$$

where $G_{1M}(E)$ is the $(1, M)$ element of the retarded Green's function matrix of the DNA molecule. $\Delta_1(= \Delta_M)$, the spectral density matrix, is related to the semi-infinite left(right) electrode Green's function matrix. The details of how Δ and $G_{1M}(E)$ may be calculated are found in [24]. Having introduced the self-energy corrections into the bare molecule Green's function, electronic Green's function of the DNA molecule in the CNT/DNA/CNT sandwich is defined as

$$G^{-1} = G_m^{-1} - \Sigma^{\mathrm{L}} - \Sigma^{\mathrm{R}}, \tag{10}$$

where G_m^{-1} and $\Sigma^{\mathrm{L(R)}}$ are the retarded Green's function of the bare DNA molecule and the left(right) SWNT self-energy matrix, respectively. The operator of the retarded Green's function of the bare molecule is given by

$$G^m = (1z - H_{\mathrm{DNA}})^{-1}; \quad z = E + i0^+, \tag{11}$$

in which H_{DNA} represents the Hamiltonian of the bare molecule and 1 stands for the identity matrix. In order to calculate the Green's function matrix element $G_{1M}(E)$, in eq. (9), which carries all the information about the molecular structure necessary for the conductance calculation, the partitioning algorithm proposed by Mujica *et al* has to be generalized [33] to the presented ladder model of the DNA structure. Accordingly, $G_{1M}(E)$ can be found in the matrix form as follows:

$$G_{1M}(E) = [G_{\mathrm{eff}}]_{1M}^{-1} = \begin{bmatrix} G_1 & T_1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ T_1^+ & G_2 & T_2 & 0 & \vdots & \vdots & \vdots & \vdots \\ 0 & T_2^+ & G_3 & \ddots & 0 & \vdots & \vdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & 0 & \ddots & G_{i-1} & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & T_{i-1}^+ & G_i & T_i & 0 & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 & \ddots & G_{i+1} & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & T_{M-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & T_{M-1}^+ & G_M \end{bmatrix}_{1M}^{-1}, \tag{12}$$

where G_i describes the Green's function of the ith cell. Thus

$$G_1 = \begin{bmatrix} E_{11} & t & 0 & 0 \\ t & E_{12} + i\Delta_{12} & t_{\mathrm{GC}} & 0 \\ 0 & t_{\mathrm{GC}} & E_{13} + i\Delta_{13} & t \\ 0 & 0 & t & E_{14} \end{bmatrix};$$

$$G_M = \begin{bmatrix} E_{M1} & t & 0 & 0 \\ t & E_{M2} + i\Delta_{M2} & t_{\text{TA}} & 0 \\ 0 & t_{\text{TA}} & E_{M3} + i\Delta_{M3} & t \\ 0 & 0 & t & E_{M4} \end{bmatrix}$$

$$G_i = \begin{bmatrix} E_{i1} & t & 0 & 0 \\ t & E_{i2} & t_{\text{AT(CG)}} & 0 \\ 0 & t_{\text{AT(CG)}} & E_{i3} & t \\ 0 & 0 & t & E_{i4} \end{bmatrix}; \quad 1 < i < M \tag{13}$$

in which, with $i = 1, M$ and $j = 2, 3, \Delta_{ij} = \Delta$, the imaginary part of the SWNT self-energies, Σ, is given as

$$\Sigma^\alpha = \Lambda^\alpha - i\Delta^\alpha = \sum_{m_\alpha, m'_\alpha} (t_c)_{m_\alpha}(t_c)_{m'_\alpha} g^\alpha_{m_\alpha, m'_\alpha}; \quad \alpha = L(R), \tag{14}$$

where m_α and m'_α run over the interfacial end-atoms of the SWNTs. $g^\alpha_{m_\alpha, m'_\alpha}$ is the semi-infinite left(right) electrode Green's function matrix and expressed as [36]

$$g_{n_y, n'_y}(E) = \frac{1}{2\ell} \sum_{j=1}^{2\ell} \varphi_j(n_y) \tilde{G}^j(E) \varphi_j^*(n'_y), \tag{15}$$

where $\varphi_j(n_y) = \exp(ik_y^j n_y a)$, with $k_y^j a = \pi j l$ and $1 \le j \le 2l$. We assume the x direction to be parallel to the tube (and to the transport direction) and y to be the finite transverse coordinate.

$\tilde{G}(E)$ is the surface Green's function given by [36]

$$\tilde{G}^j(E) = \frac{E - \varepsilon}{4t_{\text{SWNT}}^2} \left(1 + i\frac{\sin(q^j_{\beta^*}a/2)}{\sqrt{((E - \varepsilon)/2t_{\text{SWNT}})^2 - \sin^2(\pi j/l)}} \right);$$

$$\beta^* = \text{sign}(E - \varepsilon), \tag{16}$$

and

$$\cos\left(\frac{q^j_\beta a}{2}\right) = -\left(\frac{1}{2}\right)\cos\left(\frac{\pi j}{l}\right) - \frac{\beta}{2}\sqrt{\left(\frac{E - \varepsilon}{2t_{\text{SWNT}}}\right)^2 - \sin^2\left(\frac{\pi j}{l}\right)}. \tag{17}$$

In general, there are $N = 2l$ atomic positions over the interfacial end-atoms of the nanotube. For an armchair (l,l) SWNT topology imposed, the number of carbon sites at the interface are $2l$. In this work we set $l = 5$.

According to the foregoing procedure, the electronic density of states (DOS) of the system is calculated. The DOS at site i is given by

$$\rho_i(E) = -\frac{1}{\pi}\text{Im}\{G_{ii}(E)\}. \tag{18}$$

Using eqs (12) and (13), the diagonal elements of the Green's function matrix are obtained as follows:

$$G_{ii}(E) = G_K; \quad K \ne 1, M,$$
$$G_{11}(E) = G_1; \quad G_{MM}(E) = G_M. \tag{19}$$

2.2 *The characteristic tunnelling time*

The important aspect of the molecular electronic structure, which has been less studied and has a strong influence on the size of the transmission, is the electronic coupling between the nanotube contacts and the DNA molecule. An expression was found, which related t_c, the coupling strength of SWNT/DNA interface to an interaction time, describing the delay by the electron tunnelling through this interface. Theoretically, the electron behaviour in a quantum mechanical system is subject to the limitations imposed by the uncertainty principle. Therefore, the study of the conductivity through the mesoscopic segments must be accurately treated in order to characterize the electron transmission in these systems. So, the characteristic interaction time, as expected, via the minimized energy–time uncertainty relation, is given by

$$\tau(E) = \frac{\hbar}{2\Delta E}, \tag{20}$$

where ΔE is the change of the electron energy E during the tunnelling process. For small ΔE, one may expand $t(E)$, the transmission amplitude, as

$$t(E + \Delta E) = t(E) + \Delta E \frac{\partial t(E)}{\partial E} + \cdots.$$

For ΔE satisfying $\Delta E(\partial t(E)/\partial E) \approx O(t(E))$, the following form will be resulted for the interaction time [39]:

$$\tau(q) = \left| -\left(\frac{\hbar}{t_{\mathrm{SWNT}}}\right) \frac{1}{t(q)} \frac{\partial t(q)}{\partial q} \right|, \tag{21}$$

where $q = (\varepsilon_0 - E)/t_{\mathrm{SWNT}}$ is set. To this end, using eqs (8) and (9) for $|t(E)|^2 = T(E)$, one may obtain the following expression for $\tau(q)$:

$$\tau(q) = \left| \left(\frac{\hbar}{t_{\mathrm{SWNT}}}\right) W(q) \right|, \tag{22}$$

where $W(q) = 1 + \left(\frac{1}{K(q)}\right) \frac{\partial K(q)}{\partial q}$ and $K(q)$ with $\chi = t_{\mathrm{SWNT}} \xi^2 (\Gamma_{1p} + \Gamma_{Mp})$ and $\delta = t_{\mathrm{SWNT}}^2 \xi^4 (\Gamma_{1p}\Gamma_{Mp} - \Gamma_{1M}\Gamma_{M1})$ is found as $K(q) = q^2 - \chi q + \delta$. Here, $\xi = t_c/t_{\mathrm{SWNT}}$ and Γ_{ij} are the matrix elements of Green's function of the DNA molecule, which are given by eqs (12) and (13). So

$$\begin{aligned} \Gamma_{1p} &= (G_1)_{1p} = E_{1p} + i\Delta \\ \Gamma_{Mp} &= (G_M)_{Mp} = E_{Mp} + i\Delta \end{aligned} \quad p = 2,3; \quad \Gamma_{1M} = \Gamma_{M1} = 0. \tag{23}$$

Finally, the following form is obtained for $\tau(q)$:

$$\tau(q) = \frac{\hbar}{|t_{\mathrm{SWNT}}|} \left| \frac{q^2 + 2\chi(t_{\mathrm{SWNT}} - 1)q + \delta(t_{\mathrm{SWNT}} + 1) - \chi}{q^2 - \chi q + \delta} \right|. \tag{24}$$
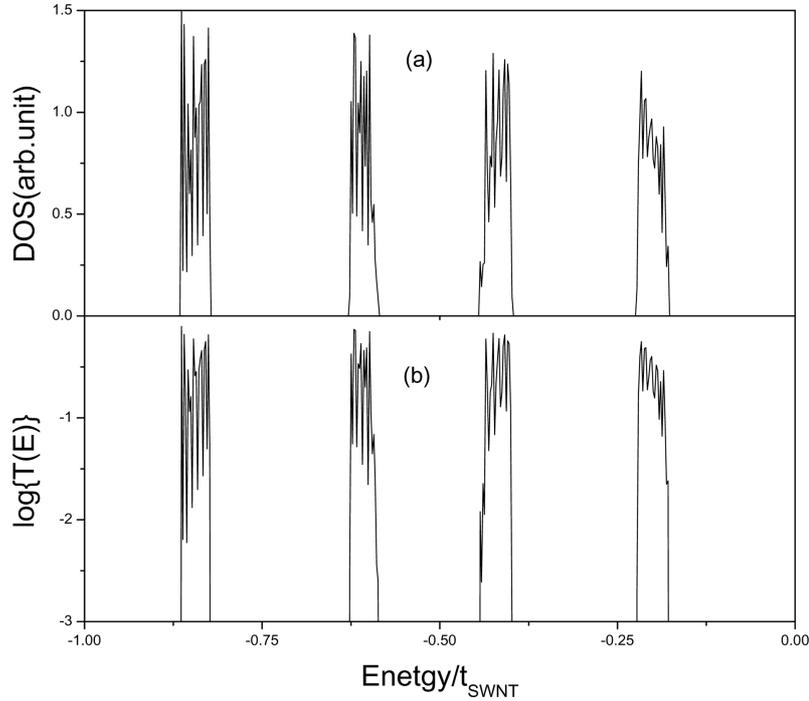
Figure 2. Panels (**a**) and (**b**) show the electronic density of states (DOS) and the logarithm of the transmission coefficient vs. the dimensionless parameter Energy/t_{SWNT} for the SWNT/DNA/SWNT system. Using the model parameters as mentioned in table 1, we set $t_{\mathrm{SWNT}} = -3$ eV, $t_c = 0.4$ eV and 32 bps for the DNA molecule. The SWNTs are considered to be armchair (5,5).

3. Results and discussion

Based on the formalism described in §2, some significant properties of the electronic conduction of the SWNT/DNA/SWNT structure were studied. To proceed, we study the electronic density of states (DOS) and the electron transmission coefficient, $T(E)$, through the DNA molecule in the foregoing structure. Panels (a) and (b) in figure 2 illustrate the DOS and the logarithm of $T(E)$ for the SWNT/DNA/SWNT structure, respectively. The DNA molecule has 32 base pairs (bps) and the SWNT electrodes are considered to be armchair (5,5). Here, the SWNT/molecule coupling strength and the hopping integral in the SWNT structure are set $t_c = 0.4$ eV and $t_{\mathrm{SWNT}} = -3$ eV, respectively. Figure 2 displays the four allowed bands for poly(GACT)–poly(CTGA) structure, which are separated, from left to right, by the relatively broad gaps $\Delta_{\mathrm{GA}} = 0.594$ eV, $\Delta_{\mathrm{AC}} = 0.432$ eV and $\Delta_{\mathrm{CT}} = 0.525$ eV. As expected, the states in the guanine band have more contribution to the charge conduction. This may be attributed to the richness of π-orbitals on the base of guanine [22]. In addition, as mentioned in table 1, the on-site potential of guanine is lower than that of cytosine, adenine and thymine.
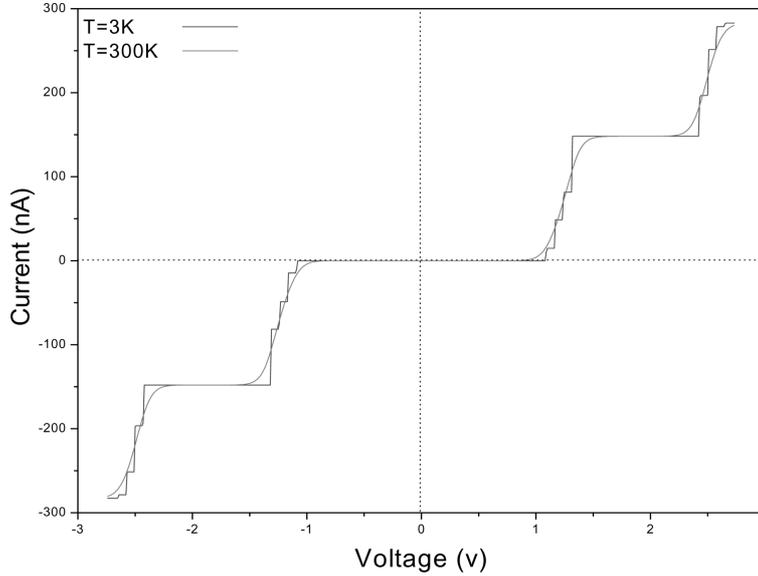
Figure 3. The current–voltage characteristics of the DNA molecule for low temperature ($T = 3$ K, step-wise curve) and room temperature ($T = 300$ K, smoothed curve) in the SWNT/DNA/SWNT system. Here, for armchair (5,5) nanotubes as the electrodes, $t_{\mathrm{SWNT}} = -3$ eV, $t_c = 0.4$ eV and 32 bps are set for the DNA molecule.

The current–voltage (I–V) characteristic of the system is shown in figure 3. To calculate the current through the SWNT/DNA/SWNT structure, we consider the standard transport formalism of electric current under an applied potential bias of V [29,39]:

$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} \mathrm{d}E\, T(E) W(E - E_{\mathrm{F}}; eV), \tag{25}$$

where $T(E)$ denotes the electron transmission coefficient of the DNA molecule in the SWNT/DNA/SWNT structure and E_{F} is the Fermi energy of the electrodes:

$$W(E, eV) = f(E) - f(E + eV), \tag{26}$$

with the Fermi function $f(E) = \left(\mathrm{e}^{\beta E} + 1\right)^{-1}$ and $\beta = (k_{\mathrm{B}} T)^{-1}$. The above Fermi function is the difference between the charge distributions before and after the transport [38,39]. The driving force, here, is the electric potential bias. Figure 3 shows the I–V characteristics for temperatures of 3 and 300 K in step-wise and smoothed curves, respectively.

The I–V curves clearly show a nonlinear dependence. Our results represent a good qualitative agreement with the electronic structure of the system (figure 2) along the zero current part of the I–V curves. In other words, despite the existence of the band gap with the average magnitude of $\cong 0.517$ eV between nucleobase bands, the low-voltage parts of the I–V curves shows a zero-current gap $\cong 2$ V,
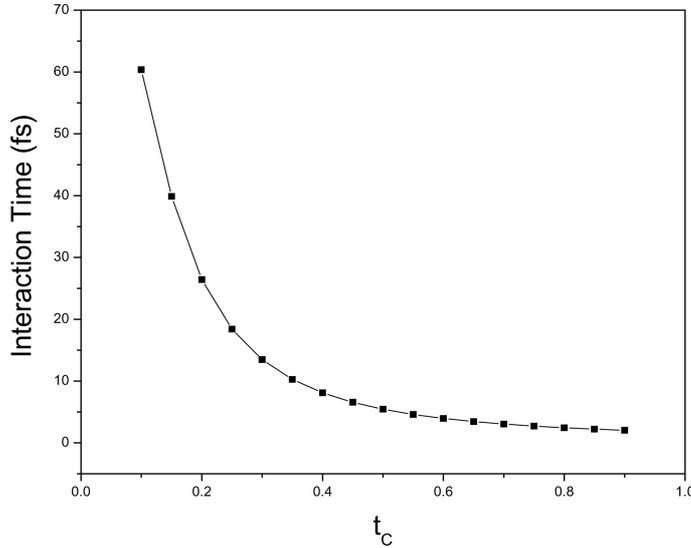
Figure 4. A plot which shows the interaction time (in units of femtosecond) vs. t_c for the SWNT/DNA/SWNT system. Using the model parameters as mentioned in table 1, we set $t_{\text{SWNT}} = -3$ eV and 32 bps for the DNA molecule. The SWNTs are considered to be armchair (5,5).

which reflect that many of the electronic states close to the gaps in the electronic structure have a very low transmission probability.

Also, the steps in the I–V curve, at low temperature, may be explained as the result of the fragmented electronic structure of the system. However, as the temperature increases, this feature is modified, whilst at higher temperatures, the step-wise part of the I–V curve is smoothed, as expected.

Using eq. (24) and considering the electrons with energies near Fermi energy (E_{F}), figure 4 shows the results of the numerical calculations for $\tau(q_f)$ with $q_f = (\varepsilon_0 - E_{\text{F}})/t_{\text{SWNT}}$ vs. different values of t_c for a DNA molecule with 32 bps. From figure 4, the strong dependence of $\tau(q_f)$ on the magnitude of t_c can be clearly seen. We see that the interaction time $\tau(q_f)$ decreases rapidly when the coupling strength of the SWNT/DNA interface, i.e., t_c increases and will be relatively constant and approaches zero for $t_c \geq 0.4$ eV. In fact, increasing t_c to the values more than 0.4 eV leads to a considerable enhancement of the conductance of the system. Our results show, once t_c drops below ≈ 0.4 eV, that a significant retardation occurs in the electron transmission at energies near the Fermi level (E_{F}). It explains the additional time it takes to transmit an electron through the SWNT/DNA interface.

Figure 5 illustrates the differential conductance of the system for some selected armchair nanotubes with different tube diameters as the electrode. We find that, as the tube radius (R) increases, the conductance of the system considerably increases. Compared with the most experimentally observed carbon nanotube sizes, there is a tiny gap in the armchair nanotube types which arises from the curvature effects [40]. Thus, the increase of the tube diameter gives rise to the decrease of the resistance
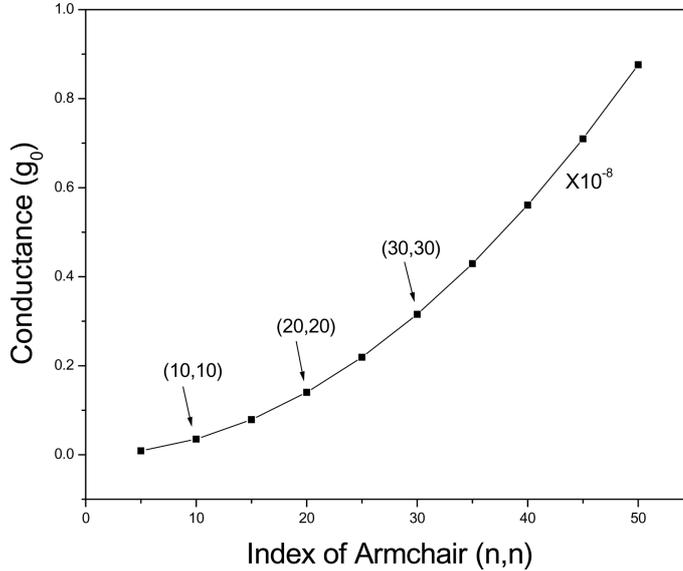
Figure 5. The differential conductance (in units of g_0) vs. the tube diameter of electrodes with $t_{\text{SWNT}} = -3$ eV, $t_c = 0.4$ eV and 32 bps for the DNA molecule in the model structure.

[41] and also the decrease in the gap as $1/R^2$ [42] and causes a large enhancement in the conductance of the system.

The calculations of $\tau(q_f)$ for the DNA model molecules have been done with different number of cells. In other words, the behaviour of the interaction time $\tau(q_f)$ has been studied for the DNA molecules of different lengths. As expected [27], figure 6 shows, when the number of cells, in the presented model for the DNA increase, the interaction time increases linearly. In this way, the number of cells has been increased from 15 to 160.

4. Conclusion

Some significant electronic conduction properties of the poly(GACT)–poly(CTGA) DNA molecule in the SWNT/DNA/SWNT system have been studied using the methodology described in §2. In the framework of the ladder model, we consider the DNA molecule with 32 base pairs as a planar molecule containing M cells and four further sites in each cell, sandwiched between two semi-infinite armchair single-walled carbon nanotubes as the nanoelectrode. Having calculated the I–V characteristics, our results suggest a good agreement with the electronic structure of the DNA in the ladder model. Also, an interaction time which explains the additional time it takes to transmit an electron through the SWNT/DNA interface in SWNT/DNA/SWNT structure has been calculated. Our results show that, in the presented model, the interaction time increases linearly with the cell number of the DNA. In addition, we find that the increase of the tube
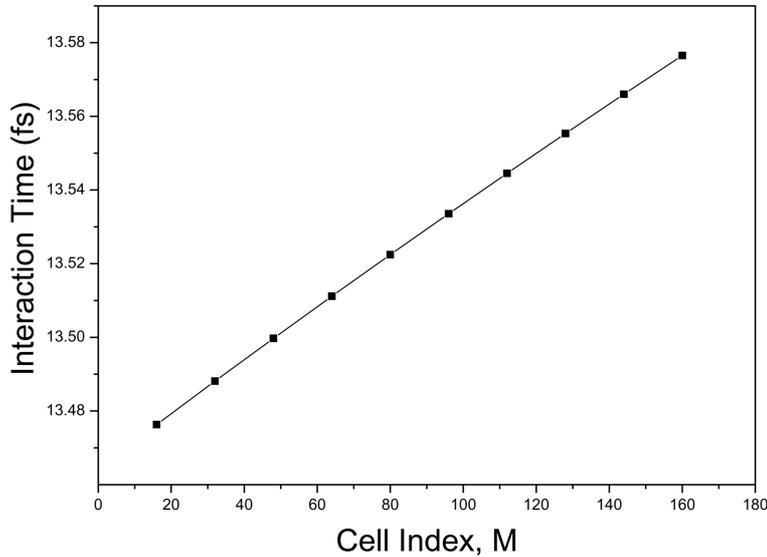
Figure 6. A plot displaying the linear increase of the interaction time (in femtosecond) as a function of cell number of the DNA ladder model. Using the model parameters of table 1, we set $t_{\mathrm{SWNT}} = -3$ eV and $t_c = 0.4$ eV. The SWNTs are considered to be armchair (5,5).

diameter of the electrodes gives rise to a large enhancement in the conductance of the system.

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