I-V characteristic of Poly(dA)-poly(dT) DNA molecule: the role of internal electric field

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Abstract. The effect of an internal electric field built up along the Poly(dA)-poly(dT) DNA molecule on the electron transport in the molecule has been studied. The electric field dependent electron hopping amplitude has been used in the tight-binding Hamiltonian model of a Poly(dA)-poly(dT) DNA molecule. Green’s function technique is used in calculating electron transmission probability, which is then used for computing current as a function of voltage by employing the Landauer-Büttiker formalism. It is observed that the internal electric field can cause the current decreases with voltages. The current reaches its maximum at a lower voltage as the internal electric field increases.

1. Introduction
Since proposed by Eley and Spivey in 1962 [1] that the possibility of DNA conduct electric current, the charge transfer, as well as transport property of the molecules remains an open question. It has been reported that DNA can behave ohmic-like, insulators, and semiconductors, even proximity induced superconductors. Recently, Daraghma, Talebi, and Periasamy proposed using a gold-DNA Schottky junction structure for investigating the charge transfer mechanisms of DNA to grabs a better understanding of DNA electronic properties [2]. The interest in understanding the charge transfer and transport property of DNA molecule stem not only understanding a biological phenomenon that may involve charge transfer or transport process [3], as an example self-repairs process in DNA itself, but also on the hope of using this molecule in electronics devices, such as non-resonant tunnelling diode [4].

Researchers developed many models for understanding the behaviour of charge conductance in DNA. Neglecting the three dimensions nature of DNA molecule, one built a one-dimensional model in which each base-pairs is assumed to be one site. Others developed static models, in which the soft and twisting nature of the molecule is not taken into consideration, such as fishbone model and ladder model [5]. In the dynamic model, the internal twisting vibration is also considered [6]. Even though many factors have been brought into consideration in the theoretical model, such as the presence of a medium, bases mismatch, etc, the role of an internal electric field which is the result of a voltage difference between metallic electrodes at both ends of DNA molecules, is rarely considered. In the model, it is usually assumed that the potential drop only at contacts such that the electric field inside the molecule is zero.

In this research, the effect of an internal electric field in the molecule which is induced by the voltage on the electrical properties of poly(dA)-poly(dT) DNA molecule will be studied theoretically. The electric field is considered modifying the magnitude of electron hopping constant in the tight-binding Hamiltonian scheme. Green’s function technique will be employed in obtaining the
transmission probability which will be used in calculating current at a given voltage using Landauer-Büttiker formalism [7]. The result shows that as the internal electric field increases, at a certain voltage the current will start to decreases.

2. Method

2.1 Theoretical model

In this study, we assume that the electric field influences electron charge transport through the hopping constant. Miller-Abraham formula [8] is used in calculating the electron hopping constant in the presence of an electric field. In the case of the electric field with amplitude $E$ situated along the DNA helix axis and temperature $T$, the electron hopping constant from site $i$ ($z$ coordinate of site $z_i$) to site $j$ ($z$ coordinate of site $z_j$) can be written as [10]

$$t_{ij} = \begin{cases} t_0 \exp \left( \frac{qE}{\xi k_B T} (z_i - z_j) \right); & \text{if } (z_i - z_j) < 0 \\ t_0; & \text{otherwise} \end{cases}$$

(1)

where $t$ is electron hopping constant, $q$ is the electron charge, $k_B$ is Boltzmann constant, and $\xi$ is the dielectric constant of the DNA. The electric field in the DNA can be varied by tuning the dielectric constant.

The DNA molecule which consists of Adenine and thymine bases, as well as sugar-phosphate backbone bond, is represented by four strands. The sugar-phosphate backbone bond forms the two outer strands, the adenine base and its complement form each of the two inside strands, respectively. A charge can travel along the strands and between adjacent strands, represented by a line in figure 1. The Hamiltonian model for the molecule in tight-binding approximation can be written as

$$H = \sum_{i=1}^{L} \sum_{\tau=1}^{4} \left\{ \epsilon_i^{\tau} + \phi_i^{\tau} \right\} |i, \tau\rangle \langle i, \tau| + \sum_{\sigma=1}^{4} \left[ t_{\tau\sigma}^{\tau+1} |i, \sigma\rangle \langle i+1, \sigma| + t_{\tau\sigma}^{\tau+1} |i, \sigma\rangle \langle i, \sigma| \right]$$

(2)

In the equation above, $L$ is the length of the molecule measured in base-pairs which is set 32 bps. Symbol $i$ and $\tau$ ($\sigma$) respectively represent site and strand where the electron at. Onsite energy at a particular site and strand is given by $\epsilon_i^{\tau}$. Detail of the parameter in the equation can be found in ref [10] and references therein.

![Figure 1](image-url)
Figure 2. The electrical current in poly(dA)-poly(dT) DNA molecule under the influence of the internal electric field for several electric field strength calculated at temperature 77 K and twisting motion frequency 5.12 meV. The inset is the I-V characteristic at low voltage and the vertical red dot line is for reference.

2.2. I-V characteristic calculation
In the model, the DNA molecule is placed in between two metallic electrodes, as illustrated in figure 1. The left and right electrode are also written in tight binding Hamiltonian approach. The onsite energy in metallic electrode at each end of the molecule is set to 8.45 eV. The Green’s function of this system can be stated as

\[ G(\varepsilon) = [(\varepsilon + i\eta) - H - \Sigma]^{-1}. \]  

(3)

In Eq. (3), \( H \) is the Hamiltonian of the DNA molecule. The electron energy is represented by \( \varepsilon \) dan \( \eta \) is a small positive number. The molecule-electrode contact is included in the calculation as \( \Sigma \). The molecule-electrode coupling is represented by molecule-electrode hopping constant which is taken to be 0.75 eV, equal to the hopping constant in metallic electrodes.

The transmission probability can be obtained from Green’s function through the relation [9]

\[ T_{pq} = Tr[\Gamma_p G_{pq} \Gamma_q G_{pq}^\dagger], \]  

(4)

where \( \Gamma \) is the energy broadening caused by the presence of the metallic electrodes. This broadening can be obtained from self-energy \( \Sigma \) using

\[ \Gamma_{p,q} = i(\Sigma_{p,q} - \Sigma_{p,q}^\dagger). \]  

(5)

One can calculate the current flowing through the molecule at a given voltage by employing Landauer-Büttiker formalism [9] which relates the transmission probability and current. The relation can be stated as
\[ I = \frac{-e}{\hbar} \int dE T(E) \left[ f_L(E) - f_R(E) \right]. \]  

(6)

It is clear from Eq. (6) that the current depends on the charge density on the left and right electrodes which are represented by Fermi-Dirac distribution \( f(E) \).

3. Result and Discussions

The role of an internal electric field on the transport properties of 32 bps poly(dA)-poly(dT) DNA molecule is studied through the I-V characteristic. The I-V characteristic is calculated by using the relation between the internal field and the voltage at contacts as \( E_{\text{internal}} = \frac{E}{\xi} = \frac{V}{\xi d} \), where \( V \) is the voltage, \( d \) is the length of the DNA and \( \xi \) measures how strong the external electric field induces the internal electric field, smaller \( \xi \) means larger internal electric field. Figure 2 shows the I-V characteristic calculated by considering the internal electric field and twisting motion of molecule with frequency 5.12 meV at temperature 77 K. As can be seen in the figure, for a weak internal electric field (\( \xi = 999 \)), the current does not immediately increase as the voltage is turned on. It starts increasing after the voltage reaches a certain threshold value. As the voltage increases beyond the threshold voltage, current increases significantly, and eventually it reaches a maximum value and then starts to decreases slowly, the differential resistance becomes negative. A similar trend is also observed at the I-V characteristic calculated for a stronger internal electric field (\( \xi = 105, 200, 400, \) and 700). The effect of the internal electric field on the threshold voltage and the current at low voltage, in general, is insignificant. However, at voltages larger than the threshold voltage, stronger internal electric field results in the lower current. In addition to lowering the voltage of maximum current, the increase of the internal electric field makes the decrement of current with voltage more prominent. The trend of negative differential resistance (NDR) is also observed by other theoretical work in which the perturbative strain- and tilted angle-dependent DNA helix conformation together with the theories of Slater–Koster is brought into consideration [11]. According to our model, the NDR behaviour can be manipulated by tuning the internal electric field strength.

![Figure 3](image-url)

**Figure 3.** Transmission probability calculated for temperature 77 K and twisting motion frequency 5.12 meV at several voltages: (left panel) higher internal electric field, \( \xi = 105 \), and (right panel) high internal electric field, \( \xi = 200 \).
To see how the trend in the I-V characteristics emerges, we calculate the transmission probability at several voltages for different internal electric field strength. Figure 3 shows the transmission probability calculated for two internal electric field strength, $\xi = 105$ (left panel) and $\xi = 200$ (right panel). The transmission probabilities are calculated at voltage closed to the voltages of maximum current, around 1.45 V for $\xi = 105$ and 1.55 V for $\xi = 200$. The transmission probability calculated show a similar feature, but different in magnitude. The transmission probability decreases with the increase of the internal electric field. Therefore, the current magnitude also decreases. The transmission probability also decreases with the voltage. At voltage larger than the voltage of maximum current, the increase of states involved in the transport process does not enough to compensate for the decrease in transmission probability. It results in the NDR feature of the I-V characteristics above the voltage of maximum current.

4. Conclusion
The I-V characteristic and transmission probability of the poly(dA)-poly(dT) DNA molecule have been calculated by bringing into consideration the presence of internal electric field built in the molecule due to the external electric field. Around the threshold voltage, in low voltage region, the current almost is not affected by the presence of the internal electric field. However, in higher voltage region the current is significantly affected by the internal electric field, stronger internal electric field results in a lower current. For all internal electric field used in the calculation, independent of the electric field strength, after the threshold voltage, the current increases until reaching its maximum, and after that the current start to decrease. This NDR feature may be due to with the increase in voltage, the number of states involved in the transport process also increase, but it does not enough to compensate the decrease in transmission probability of the states.

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