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The electrical properties of poly(dA)-poly(dT) DNA molecule: electrical current influenced by magnetic field and electric field

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Abstract. This theoretical study aims to determine the electrical properties of poly(dA)-poly(dT) DNA molecule under influence of electric and magnetic fields as external disturbances. The electrical properties of the DNA is investigated using a tight-binding model in the second quantization form. Then, the Landauer-Buttiker formalism is used in calculating electric current from the transmission probability which is calculated using the green function approach. While the external interference is considered by modelling the magnetic dependent hopping phase and the electric field dependent hopping amplitude in the tight binding Hamiltonian. The calculation results shows that the electric field applied along the DNA decreases sharply the peak of the transmission band. This means that the electric field significantly weakening the quality of transmission in poly(dA)-poly(dT) DNA molecule. On the other hand, the increase in magnetic field results in the increment of maximum current and the decrement of threshold voltage.

1. Introduction
In recent decades, biomolecular technology research has been thriving across the field involving physicists, chemistries, biologist, and nano-engineer alike. The utilization of biomolecular technology devices has taken to a new level of the process of identifying diseases from a macro sample (blood and sputum fluid) into a smaller sample (nucleic acid and protein) [1, 2, 3]. Then, biomolecular technology has also been bringing in a small electronic device and more maximum performance [4]. There is DNA (Deoxyribose Nucleic Acid) in all organisms. It is a candidate in biomolecular technology devices. The structure of DNA was found by Watson-Crick in 1953 [5]. DNA molecule has a double helical chain that consists of two sugar-phosphate backbones and four kinds of bases, adenine, thymine, guanine, and cytosine. The combination of all DNA components creates its unique properties such as the genetic information career, self-assembly capability [4, 6], and its conductivity [7].

The characteristics of DNA molecule relating to its capability in conducting electric current is a special topic of interest for some researchers. It was first discovered by Eley and Spivey [7] in 1962 that DNA can conduct electric current. However, after many experiments, researchers found that DNA has varieties of electronic behaviour: ohmic-like [8], insulators [9,10], and semiconductors [11,12]. The researchers guessed that diverse conductivities of DNA molecules may be caused by internal and external factors. In order to understand the role of these factors, researcher study this molecule by making model in the hope of finding alternative applications in future technology. The charge movement in DNA molecule is modelled in one-channel model and two-channel model without considering the role of sugar-phosphate backbone. Bringing the backbone into consideration,
researches develop fishbone model and ladder model. In addition to the charge movement in DNA, researchers investigate the DNA transport by considering the effect of temperature, too. However, the role of electric field and magnetic field in the transport process in poly(dA)-poly(dT) molecule is rarely explore. The understanding of the capability of a DNA molecule conducting current in all aspects including the presence of electric and magnetic fields is important for application of the molecule in molecular electronics devices. Therefore, it is necessary to investigate the role of electric and magnetic fields in the electron transport process in poly(dA)-poly(dT) DNA molecule.

In this research, authors study theoretically the electrical properties of poly(dA)-poly(dT) DNA molecule in the presence of external electric and magnetic field. The pathway of electron movement in DNA is represented using the backbone in ladder extended model. The model used is written in tight-binding Hamiltonian approach. For tight-binding parameters, the author uses other researcher’s parameters such as hopping constant [13], onsite energy [14], and electron-vibration coupling constant [13,14]. Electric current at a given voltage is calculated using Landauer-Buttiker’s formalism [15] from transmission probability which is calculated using the green function approach.

2. Method

2.1. Theoretical Model
Poly(dA)-poly(dT) DNA molecule is a synthetic molecule which consists of nucleobases adenine and thymine. These two bases are arranged on two different strands. The bases in a strand are connected by backbone which is situated outside the DNA molecule. Then, the poly(dA)-poly(dT) DNA molecule is positioned in between two metallic electrodes which have different voltages. Schematic diagram of the system is depicted in figure 1. In this setup, the leads function as the electron reservoir for the transport through DNA molecule. Electron as a charge career can move between bases in intra-strand and inter-strand fashions, between backbone sites, and between a base and backbone site, as illustrated using black lines in figure 1. The model of charge migration in the DNA molecule system is represented in tight binding approach in the second quantization form by

\[ H = \sum_{i=1}^{N} \{ \sum_{\tau=1}^{4} (e_i^\tau + \phi_i^\tau) |i, \tau > < i, \tau| + \sum_{i=1}^{4} \left[ t_{i,i+1}^{\tau,\tau+1} |i, \tau > < i, \tau+1| + t_{i,i+1}^{\tau,\tau-1} |i, \tau > < i+1, \tau-1| \right] \}, \]  

with

\[ \phi_i^\tau = b_{i-1,i}^\tau (\cos \Delta_{i-1,i}^\tau - \cos \varphi_{eq}) + b_{i,i+1}^\tau (\cos \Delta_{i,i+1}^\tau - \cos \varphi_{eq}), \]

the effect of internal twisting vibration of DNA molecule, where

\[ \Delta_{i-1,i}^\tau = \varphi_{eq} - (\varphi_{i-1}^\tau - \varphi_i^\tau) \]

and

\[ \Delta_{i,i+1}^\tau = \varphi_{eq} - (\varphi_i^\tau - \varphi_{i+1}^\tau). \]

In the previous equations, i, \tau, t, \epsilon, and b are symbol of a site, bases and backbone strand, hopping constant, onsite bases, and electron-vibration coupling constant. While \( \varphi_{eq} \) is twisting angle created by two bases at equilibrium which is set 36º, \( \varphi \) is instantaneous twisting angle of a base measured relative to its equilibrium position. As explained in ref. [13], the twisting vibrational motion of base pair influences electron hopping amplitude. The total number of bases pairs in the DNA, DNA molecule length, in this study in 32 DNA bases pairs, represented by L.
Figure 1. Poly(dA)-poly(dT) DNA molecule model in between two leads. Blue rings, yellow pentagon, and green hexagon are backbone, adenine, and thymine. While the black lines are the path of charge movement.

In this study, the external magnetic field and electric field are arranged parallel to the DNA chain. These fields influence charge migration are represented in two different mechanisms. The electric field affects the magnitude of hopping amplitude. Ling et al. [16] state that under the influence of external electric field $E$, hopping amplitude of electron in a distance $R_{ij}$, distance between site-$i$ and site-$j$ in organic semiconductor molecules can be written as

$$
t_{ij} = t_0 \exp \left( - \frac{(\varepsilon_i - \varepsilon_j) + q |R_{ij}| \cdot E}{k_B T} \right); (\varepsilon_j - \varepsilon_i) > q |R_{ij}| \cdot E \tag{5}
$$

$$
t_{ij} = t_0 \quad ; (\varepsilon_j - \varepsilon_i) \leq q |R_{ij}| \cdot E \tag{6}
$$

Different with external electric field, the external magnetic do not affect the magnitude of hopping amplitude but it changes hopping amplitude phase. Rudolf Pierls explains the change by adding hopping phase constant correction [17]. The change in phase experienced by an electron moving between $r$ until $r+\Delta$ under influence of magnetic field represented by $A$, potential vector integral, can be written as $\Phi_{r,r+\Delta} = \int_{r}^{r+\Delta} A \cdot dl$. Therefore, in the magnetic field the hopping amplitude transform as follow.

$$
t_{ij} \rightarrow t_{ij} e^{-i\theta} \tag{7}
$$

2.2. Calculation of Transmission Probability and Current
In the Landauer-Buttiker’s formalism [15], electrical current through a sample depends on charge transmission probability and the different of charge population between both ends of the DNA sample as in equation (9).

$$
I_p = \frac{-e}{h} \sum_q dE \ T_{pq}(E) [f_p(E) - f_q(E)] \tag{9}
$$

The notations of $f_{p,q}(E)$ and $T_{pq}$ are Fermi-Dirac distribution at both sides of the DNA chain and transmission probability. The relation [15] of transmission probability and Green’s function can be state as
\[ T_{pq} = Tr[\Gamma_p G_{pq} \Gamma_q G_{pq}^\dagger], \]  
\[ \text{where } G \text{ and } \Gamma \text{ are Green's function and broadening function due to self-energy of the leads, respectively. The broadening can in term states of self-energy } \Sigma \text{ as} \]
\[ \Gamma_{p,q} = i(\Sigma_{p,q} - \Sigma_{p,q}^\dagger). \]

3. Result and Discussion

The transmission probability calculated in energy range of 7.35 -10.65 eV using Fermi energy 8.45 eV and electrode-molecules coupling constant 0.75 eV is shown in figure 2. The figure shows that there are three transmission bands in each graph, in the energy range of around 7.6 – 8.0 (band 1), 8.65 – 9.25 (band 2), and 9.8 – 10.45 (band 3). The electric field (\( E \)) is represented by voltage (\( V \)), \( E=V/(95d) \), \( d \) is the length of the DNA chain. Transmission probability calculated for various electric fields, 0.1 V, 0.5 V, 0.7 V, and 1.0 V, and magnetic field of 3 T are shown in figure 2(a). The influence of the electric field in transmission probability of a poly(dA)-poly(dT) DNA molecule is observable. It significantly weaken the transmission probability, especially at its high peaks. It does not only reduce the high of the transmission peaks but also tends to narrow the transmission bandwidth which results in band gaps broadening. The two indicators, reduction of peaks high and narrowing transmission bandwidth, indicate that the electric field causes a decreasing in the number of states involved in the transmission process.

![Figure 2](image-url)
Figure 3. Electrical current in poly(dA)-poly(dT) DNA molecule under the influence of external magnetic field calculated at temperature 77 K and twisting motion frequency 5.12 meV.

Furthermore, by varying the magnetic fields, 1 T, 3 T, 5 T, and 9 T, transmission probability is calculated at voltage of 0.3 V. It is shown in figure 2 (b). The transmission probabilities in the figure have similar shape. The most obvious differences are observed at the band edges around the energy of 8.0 eV, 8.7 eV, and 9.4 eV. Around these energies, the maximum transmission probability increases by the increment of magnetic field. The increment of transmission probability around the band edges is accompanied by the tendency of band gap narrowing, especially at band gap around the energy range of 8.0 – 8.63 eV (first gap). It is clear that the phase change due to magnetic field shifting the state with high transmission probability as well as increasing the number of such states, as in the energy range of 8.61-8.67 eV. The shifting of the hopping phase induces the range changing of the hopping wave function [17]. Constructive interference generates new state transmission. In contrast, destructive interference destroys state transmission.

The effect of external electric and magnetic fields on the transmission probability discussed above shows up in I-V characteristic of poly(dA)-poly(dT) DNA molecule. Figure 3 shows I-V characteristic of poly(dA)-poly(dT) DNA molecule, which is influenced by external magnetic field, calculated at temperature 77 K and twisting motion frequency 5.12 meV. In this calculation, the magnetic fields used are 1 T, 3 T, 5 T, and 9 T. The I-V characteristics calculated at these magnetic fields show similar trend which are the current starts to increase at certain threshold and decreases after reaching a certain maximum value. Increasing the magnetic field result in lower threshold voltage and higher maximum electric current.

4. Conclusion
To sum up, the transmission probability and electric current in the poly(dA)-poly(dT) DNA molecule under the influence of the electric and magnetic field have been calculated. Variations of electric fields such as 0.1 V, 0.5 V, 0.7 V, and 1 V, have some impacts on transmission probability. The increase of electric field has significantly decreased transmission probability and slightly narrowed the transmission bandwidth. Within the model used, the electric field weaken transmission quality especially at higher voltage. It causes the decrement of current with voltage after reaching its
maximum value. Meanwhile, in the range of magnetic fields used, the increase of magnetic field result in higher maximum current and lower threshold voltage.

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