Influence of magnetic and electric field on I-V characteristic of the G4 DNA molecule

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Abstract. The I-V characteristics of G4 DNA molecule in applied magnetic and electric fields has been calculated. We use DNA molecule in the form of stacked of 32 guanine quadruplex (G4) structures. The DNA molecule is contacted to the metallic electrode at both ends. The system under investigation is modeled using tight-binding Hamiltonian approach. Magnetic and electric field affects electron hopping constant following Peierls Phase Factor and Miller-Abraham, respectively. The result shows slight current increment with the magnetic field and current increment with electric fields after certain voltage value.

1. Introduction
At this moment, science and technology are developing rapidly, particularly for nanotechnology and molecular electronic [1, 2, 3]. Various nanotechnology materials have been studied by researchers, one of which is biomolecular material. Biomolecular materials have the potential to support the development of nanoscale electronic devices. One of the biomolecular materials studied is deoxyribonucleic acid (DNA). The understanding of the electronic properties of DNA molecule has attracted a lot of attention of experimentalist and theorist [4]. DNA can be synthesized and has unique characteristics which are self-recognizing and self-assembly, in which scientists use DNA as an active element in a bottom-up nanotechnology approach [3, 5].

DNA molecule is composed of nucleotides, which are made from four unique nucleotides: adenine (A), thymine (T), guanine (G), and cytosine [6]. Four types of bases are for storing the genetic information concerning the structure and function of all living organisms [7]. A special kind of DNA molecule is composed solely of guanine nucleotides (G), G4DNA [8]. G4 DNA consists of a G-quartet arrangement, which is a planar structure of four guanines that are connected by hydrogen bonds [1].

During the past few decades, physics, chemistry, and biology communities studies focused on the nature of the transport of double-stranded DNA (ds-DNA), as one of the leading candidates for molecular electronics [8]. In this research, we studied the G4 DNA molecule. G4 DNA molecule is placed in an applied electric and magnetic field, which are set parallel to DNA symmetrical axis [9, 10]. This research aims to study electric and magnetic field influence on the electron transmission probabilityin G4 DNA molecule. The effect of electric field on G4 DNA molecule, which in turn will affect the transport properties the molecule, is rarely, if ever, studied.

The parameters considered in this paper is including frequency, temperature, electric field, and magnetic field. Green’s function method along with tight-binding Hamiltonian of DNA molecule model is used in calculating the transmission probability. The molecule model and the method for calculating electron transmission probability will be discussed in the theoretical method section. The
result of the calculation will be described and discussed in detail in the results and discussion. Then the results will be summarized.

2. Experimental

2.1 Theoretical Method

DNA model molecule used in this study is G4DNA model of 32 base pairs. The unique structure of G4-DNA consists of a stacked of G quartet. Each G quartet is a set of four G bases put in a square structure with one G at its corner and is connected with hydrogen bonds. Schematic diagram of G4 DNA is shown in Figure 1. The system can be effectively described with a tight-binding Hamiltonian model.

$$H = \sum_{i=1}^{L} \sum_{\tau=1}^{4} \left[ \left( e_i^\tau + \phi_i^\tau \right) |i, \tau \rangle \langle i, \tau | + t_{i,i+1}^{\tau,\tau} |i, \tau \rangle \langle i+1, \tau | \right] + \sum_{\tau=1}^{4} \left( B_i^\tau |i, \tau \rangle \langle i, q | + t_{i,i}^{\tau,q} |i, \tau \rangle \langle i, q | \right) + \sum_{\tau=1}^{4} \left( t_{i,i+1}^{\tau,\tau+1} |i, \tau \rangle \langle i+1, \tau + 1 | \right) + \text{h.c.} \quad (1)$$

Symbol in equation 1 can be explained as follows. L is the length of the DNA chain which is 32 G quartet. Indices i, , and q are consecutively for site index, strand index, and backbone index. Base’s onsite energy and backbone’s onsite energy are represented consecutively by parameters and . Electron’s hopping constant, which depend on electric and magnetic fields, is represented by parameter . All parameter used in this work can be found in ref. [12].

External electric field which is applied in perpendicular to the planar structure of G quartet, affect the electron hopping constant according to Miller-Abrahams[9,13]. Meanwhile, the magnetic field which is also applied perpendicular to the planar structure of G quartet, change the phase of electron hopping constant. The change in phase is called Peierls phase factor [14]. Considering these two factors, electron hopping constant from site j to site i in external magnetic and electric fields can be stated as follows

$$t_{i,j} = t_o \exp \left( t_i^\tau \int_{j}^{i} A \cdot d\vec{l} + eE_\parallel \frac{z(j) - z(i)}{k_B T} \right) \quad (2)$$

where $\vec{A}$ is potential vector and E electric field, $z(j)$ is coordinate of site j, $t_o$ is electron hopping constant without both electric field and magnetic fields. $T$, e, $h_o$, and $k_B$ consecutively are temperature, electron charge, Planck constant, and Boltzmann constant.

Figure 1. Scheme diagram of G4 DNA in the electric and magnetic fields. The black color is the strand, the blue color is the site, and the red color is guanine bases.
Green's function method is used in calculating the transmission probability of G4 DNA model. Green’s function, advance/retarded, for single particle system represented with Hamiltonian $H$ can be stated

$$G^{R/A}(E) = \lim_{\eta \rightarrow 0^+} [E \pm i\eta - H],$$

where $E$ is the energy of electron. Once the Green’s function is known, the transmission at a given electron energy can be calculated using the Fisher-Lee relation:

$$T = Tr[\Gamma_l G^R \Gamma_r G]$$

represents the coupling of the molecule to the left electrode and $\Gamma_r$ represents the coupling of the molecule to the right electrode. Function $I$ can be expressed in terms of self-energy $\Sigma$ due to left/right electrode as

$$\Gamma_{l/r} = i [\Sigma_{l/r} - \Sigma']$$

3. Results and Discussion

In this paper, we report the transmission probability calculated at two cases. In the first case, we want to study how the transmission probability change if the voltage is varied and the temperature and external magnetic field are kept constant. In the other case, we consider, instead of kept constant the magnetic field is varied and electric field and temperature are constant.
Figure 2. Electron transmission probability on 32 G quartet long G4DNA molecule calculated at temperature of 77.2 Kelvin, twisting motion frequency of 2 meV and external magnetic field of 3 Tesla for several voltages.

The first case is carried out by setting temperature, twisting motion frequency, and external magnetic field, respectively, to 77.2 K, 2 meV, and 3 T. The calculation results in this case are shown in Figure 2. As can be seen in figure, at zero voltage, the transmission probability spectrum shows two region with nonzero transmission probabilities separated by a gap, one broad band around energy range of 6.7 – 8.9 eV and one narrower band around energy of 9.4 – 9.8 eV. The gap is the region from 8.9 eV to 9.4 eV which have zero transmission probabilities. The red vertical line in the figure indicates the position of Fermi Increasing the voltage across DNA molecules, affecting the molecule manifested by the changes in electron hopping constants which are, in our model, becoming smaller. The increment of voltage is widening the gap between two bands and narrowing the band of states with nonzero transmission probability. Even though the band becomes narrower, its maximum transmission probability gets higher. Not only the maximum transmission probability gets higher, but also several other states experiences the increase in magnitude. As the center high energy band moves toward lower energy, the center of wide band moves toward opposite direction making the band edge gets closer to Fermi energy. Since the change in the transmission probability will be reflected in I-V characteristic, the electric effect on the molecule property modelled used in this study shows that the electric field can change the electrical properties. Within our model, since the band edge gets closer to the Fermi energy, at higher voltage less states with nonzero probability transmission are around the Fermi energy. Therefore less states are available for transport process.
Figure 3. Electron transmission probability on 32 G quartet long G4DNA molecule calculated at temperature of 77.2 Kelvin, twisting motion frequency of 2 meV and external electric field of voltage of 0.4 V for several value of external magnetic field.

The result of the calculation of transmission probability at constant electric field for various values of magnetic fields, the second case, are shown in Figure 3. This calculation is carried out by setting temperature, twisting motion frequency, and external electric field, respectively, to 72.2 K, 2 meV, and the voltage of 0.4 V. As can be seen in the figure, the spectrum of transmission probability at no external magnetic field is very similar to the calculation result at low voltages discussed in the previous part. The presence of external magnetic field seems to not change much the transmission probability. The presence of external magnetic field only change the phase of the electron hopping constant not its magnitude. Therefore, the external magnetic field changes the phase of electron wave function which in turn changes the magnitude of electron wave function at one sites due to interferences of several wave function which come to that site via different route. Since the phase changes due to external magnetic field is small for small distance travel, the phase different of several waves arrive at one sites is also small. This result in very small changes in the electron transmission probability with the increment of external magnetic field.

4. Conclusion
The aims of this research are to study how the magnetic and electric field influence I-V characteristic on G4 DNA molecule. The transmission probability calculated in the presence of external electric field shows that the higher the voltage, the wider the energy gap at the transmission probability spectrum. This is probably due to the electric field in the model makes the value of the electron hopping constants decreases with voltage. At the end, the effect of external magnetic field on the molecule included in the model, causes less states can be participated in the transport process. The calculation result of electron transmission probability under the influence of external magnetic field shows that the transmission probability in the range of applied magnetic field of 0 - 9 Tesla tends to be constant when the magnetic field increases. Therefore, the magnetic field influence on the transmission probability is not significant.
Acknowledgements
The author would like to thank all those who contributed to this study, both in the form of moral support, facilities, and material. Thanks to Cisco Laboratory of Department of Physic Universitas Indonesia for permission to use the laboratory. Thanks also to Universitas Indonesia for funding this study through Hibah PITTA DRPM 2018 contract number: 2259/UN2.R3.1/HKP.05.00/2018.

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