Electric and magnetic field influence on localization length G4 DNA molecule

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Abstract. Electric and magnetic field influence on localization length G4 DNA molecule has been studied. This research used G4 DNA model of 102 base pair. Localization length is calculated using the transfer matrix method. The electric field is applied in the direction parallel to DNA’s symmetrical axis. The magnetic field is applied perpendicular to DNA symmetrical axis. The results of the calculation of localization length under influence of electric field showed that the localization length decreases with electric field strength, so more electron state becomes a localized state. Other results show magnetic field has no significant effect on the spectrum of the localization length, even at large magnetic field.

1. Introduction
In the development of nanoscale electronic devices, the electronic properties of DNA have attracted attentions of many scientists [1,2]. Electronic properties of DNA molecule could depend on its structure, temperature, and environment surround it. A special kind of DNA molecule is composed of guanine nucleotides (G), G4 DNA, with its distinctive structure and self-assembling properties [3]. The nature of self-assembly is the ability of molecules to make themselves into supramolecular. The structure of G4 DNA is very stable under physiological conditions because of the quadruple-G quartet that forms quadruple-helical [4].

Many experiments and theoretical studies focused on the nature of the transport of double-stranded DNA (ds-DNA) [5,6]. In this report, we studied the G4 DNA molecule. This research uses G4 DNA molecule to study electric and magnetic field influence on the localization length. G4 DNA molecule is placed in an applied electric and magnetic field. The electric fields is set parallel to DNA symmetrical axis [7]. Whereas, magnetic field is applied perpendicular to DNA symmetrical axis [8]. The parameters contained in this paper include the electric field, magnetic field, frequency, and temperature. Localization length is calculated using a transfer matrix method by operating electron wave function to tight-binding Hamiltonian. Calculation results are discussed in detail in the results and discussion. Then, the discussion will be summarized.

2. Theoretical method
DNA model used in this study is a G4 DNA model of 102 base pairs. The unique structure of G4 DNA consists of a stacked of quartet G. Each quartet G is a set of 4 G in planar structure with hydrogen bonds. The G4 DNA in the electric and magnetic fields is described as the scheme in figure 1. The system can be effectively described with a tight-binding Hamiltonian model. Tight-binding Hamiltonian model of G4 DNA is as follows [5,8].

In equation (1), \( L \) is the DNA chain length, 102 base pairs. Indices \( q, \tau, \) and \( i \) represent backbone index, strand index, and site index, consecutively. Parameters \( e_i^q \), \( B_i^q \), and \( \phi_i^q \) respectively refer to base’s onsite energy on site \( i \)-th and strand \( \tau \)-th, backbone’s onsite energy on site \( i \)-th and
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Figure 1. Scheme diagram of G4 DNA in the electric and magnetic fields. The black line is the strand, the blue line represent the boundary of the planar structure of G4 with a guanine base (black dot) at every corner.

backbone q-th, and onsite energy change on site i-th and strand τ-th due to twisting bases twisting motion [9]. Parameter t represents electron’s hopping constant. It is dependent on temperature [10] as well as electric [7] and magnetic fields [11]. In the model, we assume that electron hopping between sites is influenced by internal electric field, which is equal in both magnitude and direction to applied electric field.

2.1. Localization Length

In this research, we calculated the localization length for studying the electrical properties of G4 DNA molecule. The matrix transfer method is used to calculate the length of localization based on the following references [12,13]. The matrix transfer method can be used to calculate the amplitude of electron wave function at a given energy from Hamiltonian equation (1). The amplitude of the wave function at site L and L-1 can be calculated using,

$$H = \sum_{i=1}^{L} \sum_{q=1}^{n} \left\{ (c_i^+ + \phi_i^+) |i, \tau \rangle | i, \tau \rangle + t_{i,i+1}^{\tau} | i, \tau \rangle | i+1, \tau \rangle \right\}$$

$$+ \sum_{i=1}^{L} \sum_{q=1}^{n} \left\{ B_i^{\tau q} | i, \tau \rangle | i, q \rangle + t_{i,i,1}^{\tau q} | i, \tau \rangle | i, q \rangle \right\}$$

$$+ \sum_{i=1}^{L} \sum_{q=1}^{n} \left\{ \left( B_i^{\tau q} + t_{i,i,1}^{\tau q} \right) | i, \tau + 1 \rangle + t_{i,i+1}^{\tau q} | i, \tau + 1 \rangle \right\} + h.c.$$ (1)

The inverse of the smallest γcl gives the localization length (λ).

3. Results and discussion

The result of the calculations in this study is the electron localization length of G4 DNA molecule with 102 base pairs. The electron localization length when electric field is applied at voltage 2 mV, 4 mV, and 6 mV can be seen in figure 2, figure 3, and figure 4, respectively. The localization lengths are calculated at magnetic field of 1 Tesla, temperature of 4.2 Kelvin, and basis twisting motion frequency of 0.51 meV. The graph in the figures is the localization length as a function of electron energy. A break on Y axis in the graph from point 102 to 200, intended to mark the limit of localized state which
Figure 2. The localization length calculated at voltage of 2 mV, magnetic field of 1 Tesla, temperature of 4.2 Kelvin, and frequency of 0.51 meV.

Figure 3. The localization length calculated at voltage of 4 mV, magnetic field of 1 T, temperature of 4.2 K, and frequency of 0.51 meV.

Figure 4. The localization length calculated at voltage of 6 mV, magnetic field of 1 Tesla, temperature of 4.2 K, and frequency of 0.51 meV.

has localization length less than the length of DNA (102 base pairs). Figure 2 shows many extended states in the energy range 6.75 eV - 8.9 eV and 9.4 eV - 9.8. The extended state can conduct electrical current since electron charge travel along the molecule. In these regions, there are also some localized states, where electron that starts traveling from one end of the DNA cannot reach the opposite end. In addition, there is a gap in the energy range of 8.9 eV - 9.4 eV. The states in the gap has really small or zero localization length. Figure 3 shows similar range of energy where the extended and localized states are. However, at this voltage more states become localized. Furthermore, as we increase electric field by increasing voltage, less extended states are observed, see figure 4. Even though the magnitude of localization length at certain energy decrease as the electric field increases, it is observed that the region of energy with non-zero localization length almost does not change. The effect of increasing the electric field changes the magnitude of localization length.

Figure 5, figure 6, and figure 7 show the effect of magnetic field on electron localization length on G4 DNA molecule. The localization lengths are calculated at applied electric field of 1 mV, temperature of 4.2 Kelvin, frequency of 0.51 meV, and three values of magnetic field. The localization length at the magnetic field of 4 Tesla, 6 Tesla, and 8 Tesla respectively can be seen in figure 5, figure 6, and figure 7. Figure 5 shows many extended states in the energy range of 7.3 eV–8.9 eV and 9.5 eV–9.8. In these two energy ranges, there are localized states such as in the energy range of 6.9 eV–
Figure 5. The localization length calculated at magnetic field of 4 Tesla, voltage of 2 mV, temperature of 4.2 Kelvin, and frequency of 0.51 meV.

Figure 6. The localization length calculated at magnetic field of 6 Tesla, voltage of 2 mV, temperature of 4.2 Kelvin, and frequency of 0.51 meV.

Figure 7. The localization length calculated at magnetic field of 8 Tesla, voltage of 2 mV, temperature of 4.2 Kelvin, and frequency of 0.51 meV.

The spectrum of localization length has a gap in the energy range of 8.9 eV – 9.4 eV. Figure 6 and figure 7 indicate similar feature of localization length to the one in figure 5. It can be said that the magnetic field influence on the electron localization length in G4 DNA molecule is minute. Even though, the magnetic field difference is quite large, magnetic field increases from 1 Tesla to 8 Tesla, the different in the localization length is hard to be observed. This is because the magnetic field in the molecule of G4 DNA only affects the phase of the electron hopping constant and this phase shift is small even for quite large magnetic field for short distance traveled by electron.

4. Conclusions
This research shows that the electric and magnetic field influence on the localization length of G4 DNA molecule. The electric reduces localization length. The greater the value of the applied electric field, then electron becomes more localized at some states. The magnetic field influence on the localization length is not significant. Although a large magnetic field has been applied, due to small change in the phase of electron hopping constant the change in the spectrum of localization length is hard to notice. There are states with the localization length greater than 102 base pairs upwards undergoes decrement in localization length.

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