The effect of twisting motion dependent diagonal hopping on the I-V characteristics of poly(dG)-poly(dC) DNA molecule

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Abstract. The effect of twisting motion dependent diagonal hopping on the I-V characteristic of Poly(dG)-Poly(dC) DNA molecule has been studied. Twisting angle dependent hopping constant is model using semi-empirical Slater-Koster theory. The I-V characteristic of DNA molecule is calculated from transmission probability using Landauer-Buttiker formalism by assuming symmetric voltage drop at the contacts. The transmission probability of charge on the molecule is calculated using transfer and scattering matrix methods, simultaneously. The calculation is carried out on 32 base pairs doubled-stranded DNA molecule model sandwiched in between two metallic electrodes. The results show that at low voltage the magnitude of current is not influenced much by the change of diagonal hopping term caused by base pair twisting motion. Larger influenced is observed at higher voltages, after decreases by increasing the coupling parameter of vibration and diagonal hopping constant up to some value, current increases. This trend is observed in the I-V characteristic of DNA molecule for all frequencies and temperatures used. Lower twisting motion frequency shows larger influences of diagonal hopping term on the current than the one at higher frequencies.

1. Introduction
In 1962, Eley and Spivey [1] showed that DNA can conduct current. The electrical conduction through DNA may involve in several biological processes, such as DNA mutation [2], damage detection and self-repairing [3, 4], as well as sensor and signaling system [5, 6], as shown by several experimental results. These results shed the light on the possibility of using DNA molecules as an active element in electronic devices, such as molecular transistor [7] and biosensor [8]. Moreover, DNA molecule can be used as a template in fabricating nanoscale wire [9] for its long nature.

The possibility of using DNA in molecular scale technology increases the interest of physicists in studying the transport property of DNA molecules. However, experimental results show that DNA can be an insulator up to proximity-induced superconductor [10]. This controversy may be due to the fact that different groups measuring conductivity of DNA molecule using different types of DNA [11, 12]. It has been shown that base pairing mismatch [13] also affect the transport property of DNA. Several other factors may also lead to this controversy, e.g. medium or substrate [14, 15] and internal motion of DNA [16, 11].

The effect of internal motion of DNA in the form of base pair twisting motion has been studied by modelling electron hopping term in single channel effective tight binding Hamiltonian model changes as cosine the twist angle [14]. In this paper, two channels model is used, with electron hopping terms...
following semi-empirical theory of Slater-Koster [10]. This paper will be focused on the effects of twisting motion dependent diagonal hopping on the I-V characteristic of 32 base pair long Poly(dG)-Poly(dC) DNA molecule. Twisting motion dependent diagonal hopping is tuned by varying the linear coupling parameter of vibration and diagonal hopping constant. I-V characteristic is calculated from transmission probability using Landaur-Büttiker formalism [17] by assuming potential drops at contact symmetrically. The transfer matrix technique and scattering matrix method are employed simultaneously in calculating transmission probability [18]. The results show the influence of the linear coupling parameter of vibration and diagonal hopping constant is strong at high voltage. It is observed that by increasing the coupling parameter up to some value, current decreases, then it increases. The molecule model used in the present work will be discussed in section 2 along with the methods of calculation. Then, calculation results will be discussed in section 3. In the last section, the conclusion of discussion will be drawn.

2. Materials and methods

In the model we used, electron can hop from a base to a sugar-phosphate as well as from a sugar-phosphate backbone to a base. Electron can also hop from a base to other base in the same strand (intra-strand hopping), in Watson-Crick base pair (Watson-Crick pair hopping). The model also considers electron can hop diagonally between two bases in different strands (diagonal hopping). Semi-empirical theory of Slater-Koster [10] gives angle dependent intra-strand, diagonal, and Watson-Crick pair hopping constant, consecutively, as shown in equation (1)

\[
\begin{align*}
\text{t}_{i,j+1}^{1,i} & = t_{i,j+1}^{p,i} \left[ 1 + \alpha_{i,j+1}^{pa} \sin^2 \left( \Delta_{i,j+1}^{1,i} / 2 \right) \right] \exp \left[ -\beta_{i,j+1}^{pa} \left( \cos \phi_{eq} - \cos \Delta_{i,j+1}^{1,i} / 2 \right) \right], \\
\text{t}_{i,j+1}^{1,k} & = t_{i,j+1}^{d,i} \left[ 1 - \alpha_{i,j+1}^{d} \cos^2 \left( \Delta_{i,j+1}^{1,k} / 2 \right) \right] \exp \left[ \beta_{i,j+1}^{d} \left( \cos \phi_{eq} - \cos \Delta_{i,j+1}^{1,k} / 2 \right) \right], \quad \text{and} \\
\text{t}_{i,j}^{1,k} & = t_{i,j}^{pp} \left[ 1 + \alpha_{i,j}^{pp} \sin^2 \left( \phi_{i} - \phi_{k} / 2 \right) \right] \exp \left[ \beta_{i,j}^{pp} \sin^2 \left( \phi_{i} - \phi_{k} / 2 \right) \right],
\end{align*}
\]

where \(\phi_{eq} = 6.73, \beta^{pa} = 1.00, \beta^{d} = 6.26, \beta^{pp} = 2.85, \) and \(\alpha^{d} = 11.5. \) \(\alpha \) , the linear coupling parameter of vibration and diagonal hopping constant, will be varied.

Twisting angle of base measured relative to its position at equilibrium is \(\varphi\). Its value is assumed following Gaussian distribution with deviation standard \(\sqrt{k_{b} T / \left(I_{n} \omega^{2}\right)}\) and zero average. \(T\) is temperature, \(k_{b}\) is Boltzmann constant, \(I_{n}\) is base moment of inertia, which assumed to be in the order of theoretical value, i.e. \(1.0 \times 10^{-44}\) kgm\(^{2}\) [19], and \(\omega\) is twisting motion frequency. 36º is taken as \(\varphi_{eq}\), the angle between two neighbouring base pairs at equilibrium. The twisting motion dependent on-site energy according to [20] can be written as \(\epsilon_{i} = \phi_{i} + b_{i}^{\varphi} \cos \left( \Delta_{i}^{\varphi} - \varphi_{eq} \right) + b_{i}^{\varphi} \cos \Delta_{i}^{\varphi} \varphi_{eq}\), where \(\Delta_{i}^{\varphi} = \varphi_{eq} - \left( \varphi_{i} - \varphi_{k} \right)\), \(\varphi\) is base on-site energy at equilibrium, 7.84 eV for G and 8.85 eV for C and \(b\) is coupling parameter between charge and base pair twisting motion.

In tight binding Hamiltonian form, the DNA molecule model can be written as follows.

\[
H_{\text{dna}} = \sum_{i=1}^{N} \sum_{j=1}^{N} \left[ t_{i,j}^{1,i} c_{i,j}^{+} c_{i,j} + t_{i,j}^{1,j} c_{i,j}^{+} c_{i,j}^{+} c_{i,j} + c_{i,j}^{+} c_{i,j} \right] + \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \left[ b_{i,j}^{k} c_{i,j}^{+} c_{i,j}^{+} c_{i,j} + b_{i,j}^{k} c_{i,j}^{+} c_{i,j}^{+} c_{i,j} \right] + \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} \left[ b_{i,j}^{k} c_{i,j}^{+} c_{i,j}^{+} c_{i,j} + b_{i,j}^{k} c_{i,j}^{+} c_{i,j}^{+} c_{i,j} \right]
\]
Figure 1. The I-V characteristic of 32 base pairs long poly(dG)-poly(dC) DNA molecule at 4.2 K, $W = 0.1$ eV, and frequency 0.51 meV for various linear coupling parameter of vibration and diagonal hopping constant $\alpha_{sl}$. In the inset is the I-V characteristic calculated at temperature 30 K.

Table 1. Parameter for electron hopping constants ($t_{x,y}$) and coupling constant between charge and base pair twisting motion ($b_{x,y}$) for tight binding Hamiltonian [20, 21].

| Base | $t_{x,y}^{pa}$ (eV) | $t_{x,y}^{sl}$ (eV) | $t_{x,y}^{pp}$ (eV) | $b_{x,y}$ (eV) |
|------|---------------------|---------------------|---------------------|---------------|
| G,G  | 0.30                | 0.14                | -                   | 0.0334        |
| C,C  | 0.38                | 0.28                | -                   | 0.0341        |
| C,G  | 0.14                | 0.27                | 0.57                | 0.0299        |

In equation 2, $\epsilon$, $B$, and $t$, consecutively, represent base on-site energy, sugar-phosphate backbone on-site energy, and electron hopping constant from one base to the other or to sugar-phosphate backbone. $N$ is the length of DNA molecule, in this case $N = 32$ base pairs. The values of $b$ and $t$ can be seen in table 1.

In this study, backbone on-site energy $B$ follows uniform distribution with average value of 9.36 eV and deviation $W$, where $W$ is energy disorder due to medium and temperature. Other parameters used in this study are metal on-site energy 8.45 eV and electron hopping constant in metal 0.75 eV. Moreover, in calculating current, Fermi energy of 8.45 eV has been used.
3. Results and discussion

The I-V characteristic of 32 base pairs poly(dG)-poly(dC) DNA molecule calculated at 4.2 K, $W = 0.1$ eV, and frequency 0.51 meV for linear coupling parameter of vibration and diagonal hopping constant is shown in figure 1. This result and other calculation results is the average of 400 twisting angle configurations. The figure shows that the variation of the linear coupling parameter of vibration and diagonal hopping constant almost does not change the current magnitude at low voltage. At higher voltage, the influence of coupling parameter is getting larger. As the coupling parameter increases up to a certain value, the current magnitude decreases. After that, the current magnitude increases and seems to saturate. The plateau in the range of 1.5 and 2.0 volt emerges due to gap on transmission probability as function of energy. Even though I-V characteristic profile is different, similar trends are observed at higher temperature as shown in the inset.

Calculated I-V characteristic at frequency 1.02 meV shows similar trend as the one calculated at 0.51 eV. However, the influence of linear coupling parameter is lesser at 1.02 meV than 0.51 meV. Calculated I-V characteristic on 32 base pairs poly(dG)-poly(dC) DNA molecule at 4.2 K, $W = 0.1$ eV, and frequency 1.02 meV for various linear coupling parameter of vibration and diagonal hopping constant is shown in figure 2. The influence of linear coupling parameter on I-V characteristic seems stronger at higher temperature as shown in the inset. The trend that the influence of linear coupling parameter on the current at higher voltage is larger is observed at all frequencies and temperature used. However, the change in current lessens with the increment of frequency as well as temperature.

![Graph](image.png)

**Figure 2.** The I-V characteristic of 32 base pairs long poly(dG)-poly(dC) DNA molecule at 4.2 K, $W = 0.1$ eV, and frequency 1.02 meV for various linear coupling parameter of vibration and diagonal hopping constant $\alpha^{\prime}$. In the inset is the I-V characteristic calculated at temperature 30 K.
4. Conclusions
At low voltage, the magnitude of current is not influenced much by the change of the linear coupling parameter of vibration and diagonal hopping constant. At higher voltage, at first current decreases by increasing the linear coupling parameter up to some value, and then it increases. Higher twisting motion frequency shows weaker influences of linear coupling parameter on the current. These trends are observed at all temperature used in the study.

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