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Direct current hopping conductance along DNA chain*

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This paper proposes a model of direct current (DC) electron hopping transport in DNA, in which DNA is considered as a binary one-dimensional disordered system. To quantitatively study the DC conductivity in DNA, it numerically calculates the DC conductivity of DNA chains with different parameter values. The result shows that the DC conductivity of DNA chain increases with the increase of temperature. And the conductivity of DNA chain is depended on the probability p, which represents the degree of compositional disorder in a DNA sequence to some extent. For $p < 0.5$, the conductivity of DNA chain decreases with the increase of p, while for $p \geq 0.5$, the conductivity increases with the increase of p. The DC conductivity in DNA chain also varies with the change of the electric field, it presents non-Ohm's law conductivity characteristics.

Keywords: DNA chain, hoping transport, DC conductivity, compositional disorder
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1. Introduction

Electron transport through DNA, first proposed by Eley in 1962,[1] is attracting a considerable amount of attention for its biological functions such as the repair mechanism after radiation damage and biosynthesis.[2,3] Recent experiments have demonstrated that there is long range charge migration along the DNA chain, and indicate that the DNA chain is a candidate for a one-dimensional (1D) molecular wire.[4,5] It is thus not surprising that DNA molecules became the subject of an intense study concerning their potency to carry an electric current,[6,7,8] and to provide a scaffold for the metal assembling of highly conductive nanowires.[9,10]

As far as electron transport through DNA is concerned, the available experimental results are still controversial mainly due to the complexity of the environment and the molecule itself. Concerning theory, the most reliable procedure to tackle these systems would be the ab initio quantum chemistry approach. However, massive numerical costs complicate its use for realistic biological systems. Recently, the energy levels and electronic states of DNA were studied,[11−15] the observed temperature-dependent conductivity in DNA was studied by considering DNA as 1D disordered system,[16] and the conduction of DNA molecules was also studied by using a charge-ladder model.[17] In addition, it is found that the introduction of long-range correlations in DNA sequences markedly changes their physical characteristics and can play a crucial role in their electron transporting.[18−20] However, the electric field dependence of the conductivity in DNA, especially the function of disorder in electronic transport of DNA chain, has hardly been studied. In this paper, we investigate the role of disorder in electron transport in DNA chain and present the temperature and electric field dependence of the conductivity in DNA, by considering that electrons may use hopping for conduction in DNA, which can be viewed as a 1D binary disordered system.

This paper is organized as follows. In the next section, we present our theoretical model based on an electronic tight-binding Hamiltonian suitable to describe DNA chain. Then we introduce the conductance formula. In Section 3 we study the temperature and electric field dependence of the conductivity in DNA, and the role of disorder in electron transport in DNA chain. Finally, the conclusions of this work are

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presented in Section 4.

2. Method of calculations

A DNA chain is a sequence of four possible nucleotides which define the structure of the amino acids to form proteins. Thus the DNA nucleotide sequences can be considered as a symbolic sequence of a four-letter alphabet, namely guanine (G), adenine (A), cytosine (C) and thymine (T). Considering the pairing of complementary bases (A with T and G with C) inside the helix, where each base is covalently bound to the backbone and bound to its complementary via hydrogen binding, we can view a DNA chain with random base pair sequence as 1D disordered systems.[19]

In order to study the electronic property of the DNA chain, we map it into a binary alphabet so that nucleotides A and T give $\varepsilon_{\rm A}$, and nucleotides C and G give $\varepsilon_{\rm B}$. Based on the tight-binding approximation and one-band approximation, the Hamiltonian is

$$H = \sum_{i=1}^{N} \varepsilon_i |i\rangle\langle i| = \sum_{i=1}^{N}\sum_{j\neq i}^{N} t_{ij}|i\rangle\langle j|, \tag{1}$$

where ε_i is the energy assigned to each random base pair site i which takes two values $\varepsilon_{\rm A}$ and $\varepsilon_{\rm B}$ with probabilities p and $1-p$, and p corresponds to the percentage of nucleotides pairs A–T, N is the number of base pairs (the length of DNA chain is $L = Na$, $a = 3.4\times10^{-10}\,{\rm m}$). Obviously, $|\varepsilon_{\rm A} - \varepsilon_{\rm B}|$ quantifies the spread of the energy distribution, namely, the degree of energy disorder W. In this paper, we assume $W = 1$, that is $\varepsilon_{\rm A} = 0.5\,{\rm eV}$ and $\varepsilon_{\rm B} = -0.5\,{\rm eV}$.[19] And t_{ij} is the electronic overlap (hopping term) between the wavefunctions of electrons centred at two neighbouring base pair sites i and j, which are assumed to be

$$t_{ij} = -2/(|i-j|+1), \quad |i-j| \leq 2. \tag{2}$$

The Schrödinger equation for the Hamiltonian (Eq.(1)) becomes

$$\begin{aligned} E_i\phi_i = \; & t_{i-2,i}\phi_{i-2} + t_{i-1,i}\phi_{i-1} + \varepsilon_i\phi_i \\ & + t_{i,i+1}\phi_{i+1} + t_{i,i+2}\phi_{i+2}, \end{aligned} \tag{3}$$

where E_i is the energy corresponding to the electron wavefunction, $|\phi_i|^2$ is the probability of finding an electron at site i in DNA random base pair sequence, and $|\varphi\rangle = \sum_i \phi_i|i\rangle$ is an eigenstate with energy E_i. Based on Dean and Martine's negative eigenvalue theorem[21] and Wu and Zheng's infinite order perturbation theorem,[22] the eigenvectors of the DNA chain can be solved. It is well known that disorder leads to localization, and each localized wavefunction has its own central localized position, and the localization length $\lambda(E_i)$ can be computed by

$$\frac{1}{\lambda(E_i)} = \lim_{N\to\infty}\frac{1}{N}\ln\left|\frac{\phi_N}{\phi_0}\right|. \tag{4}$$

The electron hopping between these localized states along the chain is responsible for the conductivity. In the following, we describe the electronic transport mechanism in DNA chains by using the simplest approach. There are only three necessary conditions for characterizing the hopping process. Under these conditions the direct current (DC) conductance can be derived, so it is referred to as electronic hopping transport conductance model of DNA chains. The three conditions are given as follows:

(1) The electrons are transported through an incoherent hopping process between two localized states with the energy interval being equal to the energy provided by the phonon and the electric field.

(2) The probability of the central position R_i of a certain localized state whose eigenvalue is E_i occupied by an electron is characterized by Fermi distribution

$$f(E_i) = \frac{1}{\exp[(E_i - E_{\rm F})/k_{\rm B}T] + 1}. \tag{5}$$

where $k_{\rm B}$ is the Boltzmann constant, T is the temperature.

(3) The jump rate for an electron to hop from one localized state to another is assumed to be[23]

$$P_{ij} = v_0\exp(-2\alpha R_{ij})\exp\left(\frac{|E_j - E_i|}{k_{\rm B}T}\right), \tag{6}$$

where v_0 is the attempt-to-jump frequency which should be a typical phonon frequency, α^{-1} is the localization length, R_{ij} is the electron hopping distance, namely $R_{ij} = |R_j - R_i|$, $|E_j - E_i|$ is the energy difference between two sites.

To calculate the DC hopping conductance we shall calculate the number of transitions from base site i to j. In the absence of an electric field there is a detailed balance, and the number is exactly equal to the number of reverse transitions. However, in the presence of an electric field an imbalance appears, and a current appears which is proportional to the voltage drop between the base sites. The positive current density from site i to j is given by[23,24]

$$J_{ij} = \frac{e^2}{k_{\rm B}T}P_{ij}f(E_i')[1 - f(E_j')], \tag{7}$$

where e denotes the electronic charge, $E'_i = E_i - \delta u_i$, and δu_i describes the energy changes affected by the electric field. For the reverse process we can get

$$J_{ji} = \frac{e^2}{k_{\rm B}T} P_{ij} f(E'_j)[1 - f(E'_i)], \tag{8}$$

so the net current density can be given by

$$\begin{aligned} J = & \frac{e^2}{k_{\rm B}T} P_{ij}[f(E'_i) - f(E'_j)] \\ = & \frac{e^2}{k_{\rm B}T} P_{ij}[E_j - E_i - (\delta u_j - \delta u_i)] \frac{\partial f(E)}{\partial E}, \end{aligned} \tag{9}$$

where $\delta u_j - \delta u_i$ can be regarded as the energy change affected by the voltage drop, namely, $\delta u_j - \delta u_i = e\varepsilon R_{ij}$, and ε is the electric field intensity. Then the total current density induced by the electronic transport is

$$\begin{aligned} J_{\rm total} == & \int \frac{e^2}{k_{\rm B}T} P_{ij}[E_j - E_i - e\varepsilon R_{ij}] \\ & \times \frac{\partial f(E)}{\partial E} {\rm d}E. \end{aligned} \tag{10}$$

In terms of the relationship between the current density and electric field intensity, we can obtain the conductivity of the DNA sequences induced by the electron hopping transport as follows:

$$\begin{aligned} \sigma_{\rm dc} = \frac{j_{\rm total}}{\varepsilon} = & \int \frac{e^2}{\varepsilon k_{\rm B}T} P_{ij}(E_j - E_i - e\varepsilon R_{ij}) \\ & \times \frac{\partial f(E)}{\partial E} {\rm d}E. \end{aligned} \tag{11}$$

3. Numerical results and discussions

In order to investigate the DC conductivity of the DNA sequence, we first study the electronic localization characteristics of the DNA sequence, and calculate the wavefunctions and the localization length of the DNA sequence with different parameter values. In Fig.1(a) we select a DNA chain with 20000 base pairs, and the nucleotides pairs A–T with probabilities $p = 0.5$.

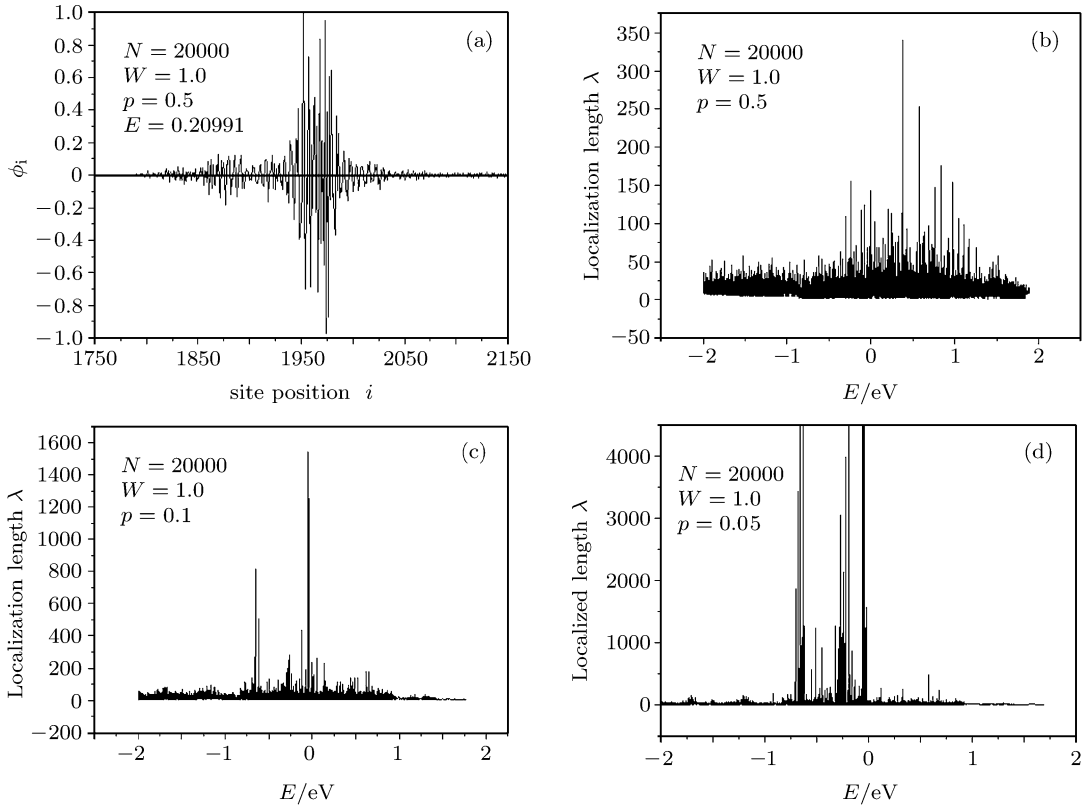


Fig.1. Electronic localization characteristics of the DNA sequence.

The wavefunction with energy $E = 0.20991\,\mathrm{eV}$ in the central band $[-2\,\mathrm{eV}, 2\,\mathrm{eV}]$ is calculated. It clearly shows that the electron wavefunctions of the DNA random base pairs sequence present the property of localization. After the electronic localized states are formed, each eigenvector has its own central localized position, and the central localized position of the wavefunction is the 1974th base pairs.

We also calculate the localization length $\lambda(E_i)$ for DNA sequence. In Figs.1(b), 1(c) and 1(d) we show the dependence of localization length on energy in DNA chain, and all the parameter values are marked in the figures. As can be seen from the figures that there exists large amount of localization states whose localization length is much less than the size of DNA chain, and the localization length presents the characteristics of the degree of proportion of nucleotides pairs dependence. That is, for $p < 0.5$, the localization length of the wavefunctions increases with the decrease of p, which corresponds to the percentage of nucleotides pairs A-T. Because the two different base pairs are randomly distributed in the chain, the probability p represents the compositional disorder in a DNA sequence to some extent. For example, when $p = 0$ or $p = 1$, the DNA chain composed of only one kind of base pairs, so it can be regarded as a perfectly periodic sequences without disorder. But when p increases from $p = 0$ to $p = 0.5$, the DNA chain varies from periodic state to disordered state, and the degree of compositional disorder increases with the increase of p. But for p increases from $p = 0.5$ to $p = 1$, the DNA chain varies from disordered state to periodic state, and the degree of compositional disorder decreases with the increase of p. That is the reason for $p < 0.5$, the localization length of the wavefunctions increases with the decrease of p.

To quantitatively study the temperature-dependent conductivity in DNA, we numerically calculate the DC conductivity of DNA chains with different parameter values. Figure 2 plots conductivity as a function of inverse temperature for $N = 20000$ and the electric field strength is fixed at $\varepsilon = 5000\,\mathrm{V/m}$ for different p. It clearly shows that the conductivity increases with the increase of temperature, and indicates that with the increase of temperature, which corresponds to an increase in delocalization, the thermal movement of base-pairs which is beneficial to the hopping of electrons will be stimulated gradually. That is, the conductivity has an activated behaviour with the increase of temperature, and indicates that hopping is mainly between nearest neighbour at high temperatures. When the temperature is rather low, the conductivity depends very weakly on temperature, and indicates that the variable range hopping is accounted for the weak temperature dependence at low temperatures, and this agrees with the early result of Yu.[16]

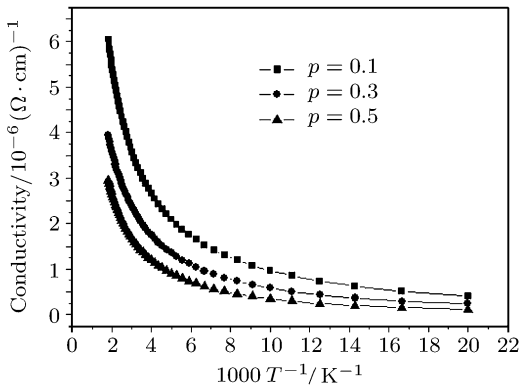


Fig.2. Conductivity of the DNA sequence versus inverse temperature.

It can also be found in Fig.2 that the conductivity of DNA chains depends on the probabilities p. In Fig.3 we show the dependence of the conductance on p for $N = 20000$ and $\varepsilon = 5000\,\mathrm{V/m}$ with different temperatures.

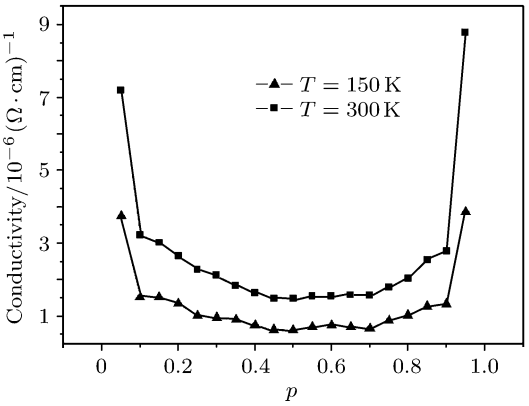


Fig.3. Conductivity of the DNA sequence as a function of p.

It can be seen that for $p < 0.5$, the conductivity of DNA chains decreases with the increase of p, while for $p \geq 0.5$, the conductivity increases with the increase of p. This implies that the proportion of nucleotides pairs plays an important role in electrons transport of DNA sequences. For $p < 0.5$, the degree of compositional disorder increases with the increase of the

percentage of nucleotides pairs A-T, and leads to increase of localization of wavefunctions and results in the decrease of jump rate. However, for $p \geq 0.5$, the degree of compositional disorder decreases with the increase of the percentage of nucleotides pairs A-T, and results in the delocalization of wavefunctions and the increase of jump rate. As a result, the conductivity of DNA chains decreases with the increase of p for $p < 0.5$, while for $p \geq 0.5$, the conductivity increases with the increase of p.

On the basis of the DC conductance formula, we can find that the conductivity of DNA sequences also depends on electric field. In Fig.4 we plot the electric field strength dependence of the conductivity of DNA sequences. It can be seen that the conductivity of system does not coincide with the regular pattern of the Ohm's law, and this excellently fits with other numerical calculations of conductivity in 1D systems.[25] As for the problem of non-Ohmic conductivity, both theoretical and experimental understanding are far from completeness, and there are still many controversial descriptions.[26−28] We think that such an unusual behaviour is due to the fact that the electron transport of DNA sequences is phonon-assisting hopping transport, that is, the electron hops between two localized states whose energy interval is provided by the phonon and the electric field. As the electric field increases, the phonon's energy dependence becomes weaker, and then the electrons have more "hopping path". For example, we assume that there are unavoidable highly resistive segments ("break") on the conducting path, as the electric field increases, the role of the breaks diminishes and eventually becomes insignificant. On the other hand, the occupation probability of a site is dependent on electric field. As a result, the DC conductivity in DNA chain varies with the change of the electric field, and presents non-Ohm's law conductivity characteristics.

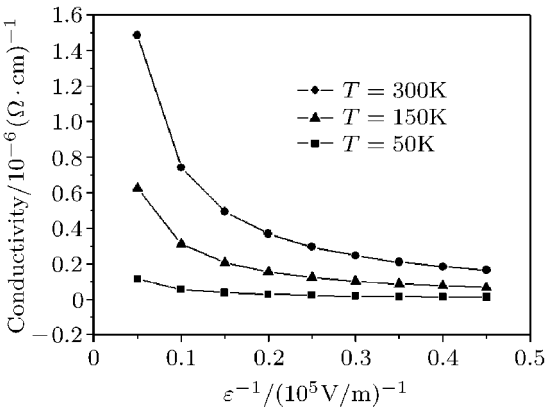


Fig.4. Conductivity of the DNA sequence as a function of electric field strength ε.

4. Summary

From the above discussion, we can draw conclusions as follows:

(1) The DC conductivity of DNA chain increases with the increase of temperature.

(2) The conductivity of DNA chain is depended on the probabilities p. For $p < 0.5$, the conductivity of DNA chains decreases with the increase of p, while for $p \geq 0.5$, the conductivity increases with the increase of p.

(3) The DC conductivity in DNA chain varies with the change of the electric field, and presents non-Ohm's law conductivity characteristics.

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