

Gap Caused by Strong Pairing in the Ladder Model of DNA Molecules *

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By directly diagonalizing the Hamiltonian of the ladder model of deoxyribonucleic acid (DNA) molecules, the density of states is obtained. It is found that DNA behaves as a conductor when the interchain hopping is smaller than twice the intrachain one, otherwise, DNA behaves as a semiconductor.

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With the development of nanoelectronics, deoxyribonucleic acid (DNA), because of its self-assembly and electronic properties as well as true nanoscale dimensions, is regarded as the preferential candidate in making nanowires.^[1-5] It is known that the DNA molecule is made of four kinds of bases of nucleotides which are stacked like an extended chain called strand, and two strands are coiled about each other to form a double-stranded helix.^[6] Moreover, base pairs of DNA obey a strict rule: adenine (A) always pairs with thymine (T) while cytosine (C) always pairs with guanine (G). Charge can transport through the bases by the overlapping of the π orbitals.^[7]

The electronic properties of DNA have been widely studied with controversial results. Experiments have shown DNA to be an insulator,^[1,8-10] a semiconductor,^[11-15] an Ohmic-like conductor,^[16] and even superconductor.^[17] In order to explain the transport properties of DNA, many models and methods have been proposed. Strictly one-dimensional tight-binding chain,^[18-20] *ab initio*,^[21] and density-functional methods^[22] give out different transport properties of DNA. The fishing backbone model,^[23] in which each poly(G)-poly(C) base pair is side-coupled to the backbone, can be used to explain the semiconductor behaviour of DNA molecules. Because of the antiresonance caused by the side-coupled G or C, the side-coupling strength can influence the gap of DNA. The two-leg charge ladder model,^[24] in which two ordered tight-binding chains are considered together with Coulomb repulsion between bases, can be used to explain the band gap of poly(G)-poly(C) DNA and the gapless feature of engineered DNA. Using effective coupling to vibration modes of molecules, the large band gap of DNA can be well explained.^[25] In addition, long-range correlation of bases can cause high conductance of DNA.^[26,27]

The ladder model of DNA was used recently to study the transport properties.^[28,29] Bands of delocalized states of DNA molecules appear due to base pairing when the interchain hopping is greater than the intrachain one.^[28] With the same model a band of extended-like states exist only for finite chain length with strong interchain coupling.^[29] However, when the interchain and intrachain hoppings are set to be 0.5 eV and 1 eV, the extended states in the ladder model does not appear.^[30] Although the base pairing can increase the localization length, the largest one is much smaller than typical sizes of samples used in various experiments. From these studies one can ask how to affect the properties of DNA by the pairing style. In this Letter, we address the influence of the strength of pairing on conducting character.

In the ladder model of DNA the hopping integrals is regarded as effective hopping. Electronic correlations^[24] or structural fluctuations mediated by the coupling to other vibrational degrees of freedom^[31] can lead to a strong renormalization of the bare electronic coupling. For the sake of simplicity, we only let the interchain hopping change, and other parameters are invariant. Density of states (DOS) of DNA is calculated by directly diagonalizing the Hamiltonian of the ladder model. It is shown that the semiconductor behaviour will appear when the strength of interchain hopping is greater than a critical value.

The Hamiltonian of ladder model of DNA is written as

$$H = \sum_j \left\{ \sum_{i=1,2} [\varepsilon_{i,j} c_{i,j}^\dagger c_{i,j} + t_0 (c_{i,j}^\dagger c_{i,j+1} + \text{H.c.})] + t (c_{1,j}^\dagger c_{2,j} + \text{H.c.}) \right\}, \quad (1)$$

where $c_{i,j}$ is the annihilation operator of electron in site j of the i th chain, $\varepsilon_{i,j}$ is the corresponding site

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energy, and t_0 (or t) is the intrachain (or interchain) hopping. In this study we use the following site energies: $\varepsilon_A = 8.24$ eV, $\varepsilon_T = 9.14$ eV, $\varepsilon_C = 8.87$ eV, and $\varepsilon_G = 7.75$ eV, the hopping parameter for adjacent nucleotides in the intrachain is taken to be $t_0 = 1.0$ eV.^[28,32] The wave function of this system can be expressed as a linear combination of electron states

$$\Psi = \sum_{i=1,2} \sum_j A_{i,j} |i, j\rangle, \quad (2)$$

where $A_{i,j}$ is the overlapping coefficient, and $|i, j\rangle$ rep-

resents the state at site j of the chain i . By directly diagonalizing the Hamiltonian in the Schrödinger equation, we obtain a series of energy levels. DOS of DNA with certain length can be obtained by counting the number of levels in small equidistant range of energy. We study the DOS of DNA with the change of strength of intrachain hopping while the other parameters are kept unchanged. The conducting behaviour of DNA is obtained when the interchain hopping is smaller than 2 eV. However, when the interchain hopping increases over 2 eV, a gap will appear in the band of DNA, which indicates the semiconductor behaviour.

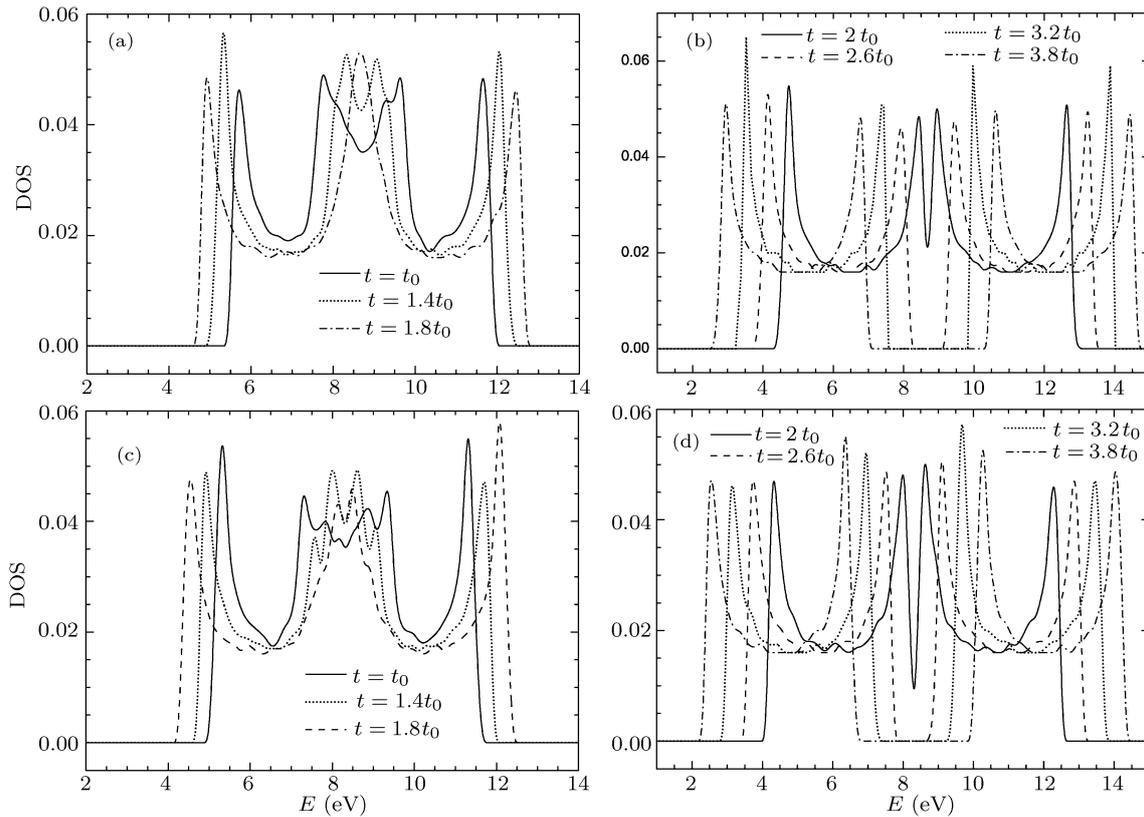


Fig. 1. DOS of DNA with 100 bases for G-C DNA [(a) and (b)] and for A-T DNA [(c) and (d)]. The intrachain hopping is set to be $t_0 = 1.0$ eV. Site energies of four bases are $\varepsilon_A = 8.24$ eV, $\varepsilon_T = 9.14$ eV, $\varepsilon_C = 8.87$ eV, and $\varepsilon_G = 7.75$ eV, respectively. Each base is randomly selected but obeys the pairing rule.

From Figs. 1(a) and 1(c) it can be found that the width of the band increases with t . When t exceeds a certain value (about 2 eV), the band starts to split into two subbands, i.e. conduction band and valence band, as shown in Figs. 1(b) and 1(d). It is supposed that DOS of DNA consists of two parts. When t is zero, the system is made up of two isolated chains. In this case the same two bands will appear, DOS of DNA is equally contributed by two chains. The two parts of DOS will start to move toward two sides with t increasing from zero. If t is not large enough, the two parts of DOS still overlap each other, therefore DNA shows conducting behaviour in a finite length. From

Figs. 1(b) and 1(d) it is found that the band starts to split when t increases to a certain value, and the band finally becomes of conducting band and valence band, respectively. We can see that in Fig. 1, the width of each subband is almost invariable although t shifts the distance of the two parts of DOS. When t increase to a critical value, the two subbands separate from each other, the semiconductor behaviour of DNA appears.

In Fig. 2, we demonstrate the gap of G-C DNA with random sequence changing with the interchain hopping. When t is smaller than about 2 eV, the gap is always zero, while the gap increases almost linearly when the interchain hopping is greater than about

2 eV. We calculate the DOS of A-T DNA and that of four-base DNA with a random sequence, which are nearly the same as that of G-C DNA. By carefully studying Fig. 1, one can find that the energy scope of DNA satisfies the simple formula

$$E \in (2t_0 \cos k + \langle \varepsilon \rangle + t) \cup (2t_0 \cos k + \langle \varepsilon \rangle - t), \quad (3)$$

where $\langle \varepsilon \rangle$ is the average value of site energy, and k is the wave vector. When t is greater than $2t_0$, the centre of energy band yields a gap, and the gap satisfies $\Delta = 2(t - 2t_0)$.

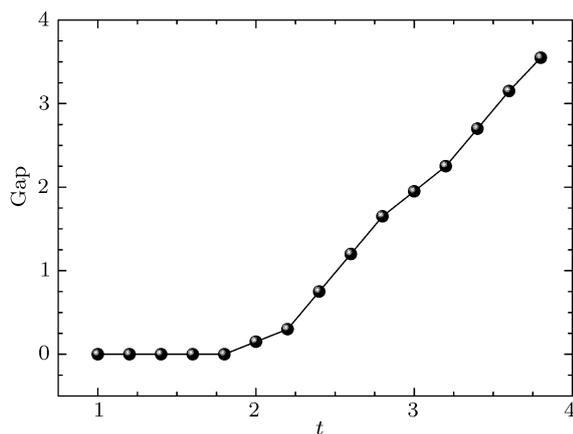


Fig. 2. Gap of G-C DNA with length 100 bases changes with the interchain hopping. Other parameters are the same as Fig. 1.

The quantum confinement can exist in systems within nanometres.^[33] We calculate the gap of DNA with different lengths (100, 500, and 1000 base pairs). It is found that the gaps for different lengths are the same, which means that the quantum confinement effect seems not to exist in DNA. As DNA can be regarded as a one-dimensional system, the changing of length of DNA do not alter the electronic structure. The gap is only decided by the base pairing.

In summary, by calculating density of states of the ladder model, we have found the semiconductor behaviour of DNA which is caused by the strong base pairing. The energy gap satisfies $\Delta = 2(t - 2t_0)$. It is expected that our simulation would be useful to explain the semiconductor property of DNA.^[11]

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