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# Effects of magnetic field and temperature on the density of states of the poly(dA)-poly(dT) DNA molecule

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**Abstract.** Charge-transport behavior in poly(dA)-poly(dT) DNA molecules is indicated by the distribution of density of states (DOS) at different electron energies. The DOS of DNA molecules in the presence of magnetic field and temperature is calculated using the tight-binding Hamiltonian and Green's function. The molecule in question consists of 32 base pairs of adenine (A) and thymine (T) in the interior, and a sugar phosphate backbone as the exterior. Electron hopping along the backbone sites is possible with this structure. The DNA molecule is connected to metallic electrodes at both ends. In the model, an external magnetic field modifies the electron-hopping constant through the Peierls transition. Temperature affects the molecule by generating a twisting motion among the base pairs. The results show that temperature and magnetic field limit the DOS of the DNA molecule for a given electron energy. Electrons can occupy all states in the energy spectrum, which are localized states, at temperatures considerably higher than zero.

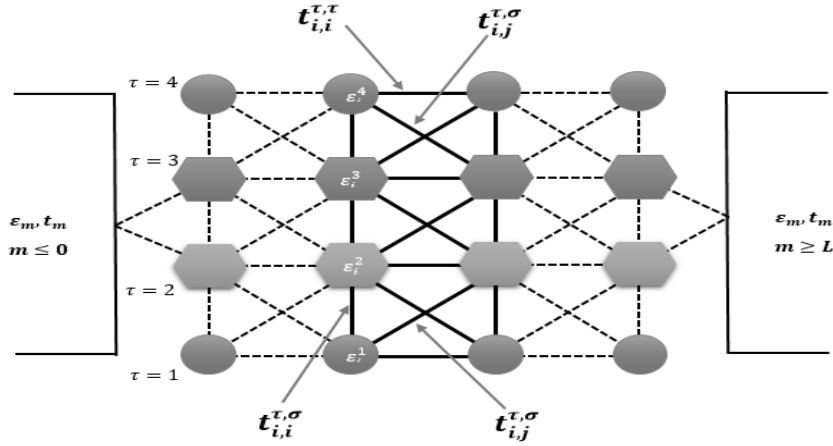
**Keywords:** density of states, poly(dA)-poly(dT) DNA, temperature, magnetic field

## 1. Introduction

DNA (deoxyribonucleic acid) is the molecule responsible for storing genetic information in all known forms of life. The primary structure of DNA consists of two chains of nucleotide polymers, the base pairs and backbone of the molecule. This structure was discovered by Watson and Crick [1]. As an important biopolymer, DNA has great potential for use in molecular-scale electronics [2] due to its unique self-assembling and self-recognizing properties. This potential for easy fabrication of specific DNA molecules has attracted research attention to the details of the charge-transport mechanisms that may be exploited in the design of electronic circuits [3,4]. Experimental and theoretical studies of charge transport along the DNA molecule suggest a variety of possible electronic behaviors. DNA molecules in different configurations, e.g., sequences and contact to electrodes, can act as insulators [5–7], semiconductors [8–10], or conductors [11,12]. This variety of functions is possible because the charge-transport mechanisms in the DNA molecule are very sensitive to intrinsic influences like the base-pair sequence, backbone structure, and hydrogen bonds between base pairs as well as extrinsic influences like the metal-molecule contacts and temperature [2].

To study a realistic model of charge transport through DNA molecule, we model the poly(dA)-poly(dT) DNA extended-ladder molecule [13], which is schematically diagrammed in figure 1. In this model, the electron-hopping amplitudes between sites up to the next-nearest neighbour are calculated under the influence of an external magnetic field and varying temperatures. In this paper, we calculate the density of states (DOS) over a range of electron energies to study the band-gap structure of the DOS spectra [13]. Furthermore, we calculate the DOS at zero temperature for several values of magnetic field as well as the DOS at zero magnetic fields for several temperatures. The band-gap structure indicates the electronic properties of the DNA molecule, and is affected by external magnetic field and temperature. In the next section, the Hamiltonian equation of DNA poly(dA)-poly(dT) and the method for calculating the DOS as a function of external magnetic field and temperature will be discussed. The results of our calculations will be discussed in the third section, and a final section summarizes the conclusions of this research.





**Figure 1.** DNA poly(dA)-poly(dT) extended ladder model. Hexagons represent thymine and adenine bases, circles represent backbone sugars. Both ends of the molecule DNA are in contact with electrodes with onsite energy  $\epsilon_m$  and hopping constant  $t_m$ .

## 2. Theoretical model

A DNA molecule with 32 base pairs of adenine and thymine is studied in this paper. Every base in this DNA structure is connected to the phosphate-sugar backbone, and each end of the molecule is connected to an electrode. The system is diagrammed schematically in figure 1. To form a realistic model of the charge-transport mechanism in DNA, electrons in the model are allowed to propagate as far as two sites away from their present site in each step of the calculation. The Hamiltonian of the poly(dA)-poly(dT) DNA molecule that used the tight binding approximation is written in equation (1).

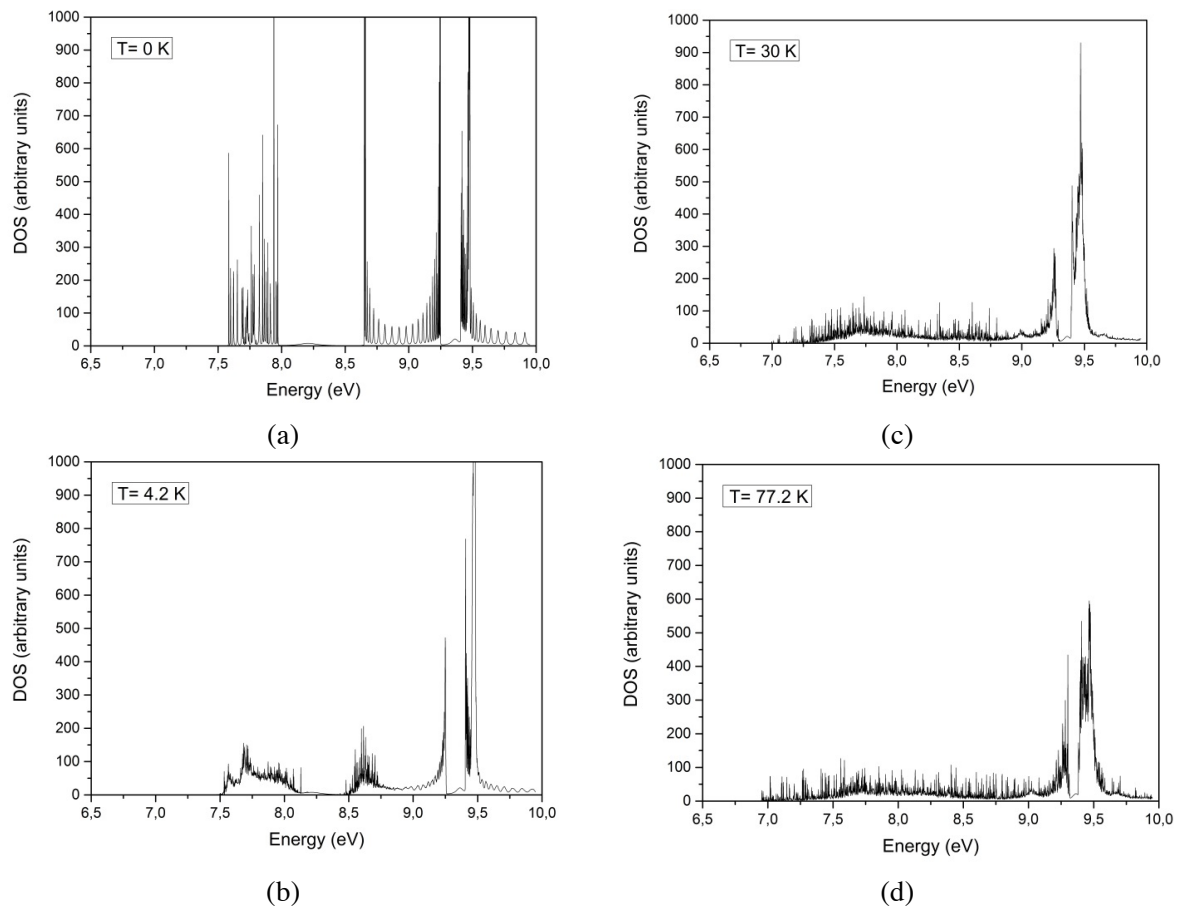
$$H_{DNA} = \sum_{i=1}^L \sum_{\tau=1}^4 \left\{ \epsilon_i^{\tau} + \phi_i^{\tau} |i, \tau\rangle \langle i, \tau| + \sum_{\sigma=1}^4 \left( t_{i,i}^{\tau,\sigma} |i, \tau\rangle \langle i, \sigma| + t_{i,i+1}^{\tau,\sigma} |i, \tau\rangle \langle i+1, \sigma| + h.c \right) \right\}$$

with  $\phi_i^{\tau} = b_{i,i-1}^{\tau} (\cos \Delta_{i,i-1}^{\tau} - \cos \varphi_{eq}) + b_{i,i+1}^{\tau} (\cos \Delta_{i,i+1}^{\tau} - \cos \varphi_{eq})$

and,  $\Delta_{i,i-1}^{\tau} = \varphi_{eq} - (\varphi_{i-1}^{\tau} - \varphi_i^{\tau})$  also,  $\Delta_{i,i+1}^{\tau} = \varphi_{eq} - (\varphi_i^{\tau} - \varphi_{i+1}^{\tau})$  (1)

The length of the DNA molecule,  $L$  is set to 32 base pairs. The sites of bases and backbone pairs are identified with the index  $i$ . The indexes  $\tau$  and  $\sigma$  represent the strand number at a site, which are 2 and 3 for the two DNA bases and 1 and 4 for the two backbone molecules. The probability of electron hopping between bases and from a base to a backbone molecule at a site is represented with parameter  $t_{i,i}^{\tau,\sigma}$ . The parameter  $t_{i,i+1}^{\tau,\sigma}$  is calculated to represent steps of the simulation. The value of each hopping constant, which depends on the angle of twist in the structure, is calculated by expansion of the Slater-Koster formula [14,15]. The symbol  $\epsilon_i^{\tau}$  is the onsite energy of base and backbone molecules at site  $i$  and in strand  $\tau$ . In this study, the energy for backbone molecule was set at 8.36 eV, and the onsite energy used for thymine was 9.06 eV and for adenine was 8.22 eV [15].

In the Hamiltonian, the effect of twisting vibrations on the base onsite energy is represented by parameter  $\phi_i^{\tau}$ . The coupling of charge and vibration is represented by the parameters  $b_{i,i-1}^{\tau}$  and  $b_{i,i+1}^{\tau}$ . Twisting vibration changes the twist angle between base pairs to the instantaneous twist angle  $\varphi_i$ . The twist angle formed by two neighboring base pairs at equilibrium is chosen to be  $36^\circ$  [14]. The instantaneous twist angle is set to follow a Gaussian distribution with average of zero and standard deviation  $\sqrt{T/f}$ .  $f$  is proportional to the square of the twisting vibrational frequency and  $T$  is the temperature (in Kelvin) [16]. In this study, the twisting vibrational frequency is set to 0.51 meV [15].



**Figure 2.** Density of states vs energy for poly(dA)-poly(dT) DNA with twisting-motion frequency 0.51 meV and magnetic field 0 T at several temperatures: (a) 0 K, (b) 4.2 K, (c) 30 K, and (d) 77.2 K.

The external magnetic field is applied alongside to the symmetrical axis of the DNA molecule. In order to simplify the problem, the Zeeman effect is ignored in the calculation. The presence of an external magnetic field affects the electron-hopping amplitudes through Peirl's phase transition [16], from  $t_{r,r+\Delta}$  to  $t_{r,r+\Delta} \exp(i e \theta_{r,r+\Delta} / \hbar)$ . The symbol  $\theta_{r,r+\Delta}$  is the line integral of the vector potential  $\mathbf{A}$  from  $r$  to  $r + \Delta$ . For an external magnetic field  $\mathbf{B}$  parallel to the DNA molecule's symmetrical axis, the line integral can be written as

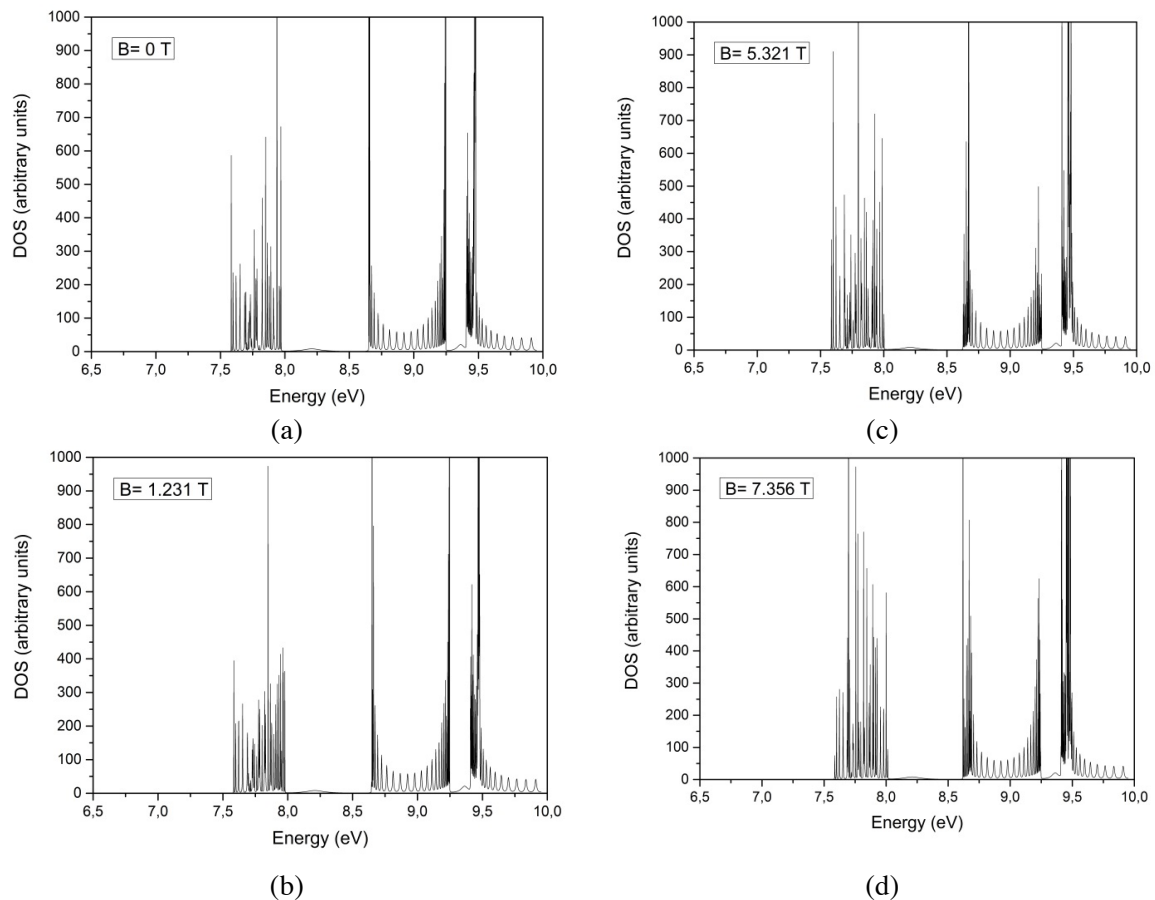
$$\int_r^{r+\Delta} \mathbf{A} d\mathbf{r} = -\frac{eB}{2\hbar} (x_j - x_i)(y_j + y_i) \quad (2)$$

where  $x$  and  $y$  represent the positions of base and backbone molecules in Cartesian coordinates.

The electronic properties of the poly(dA)-poly(dT) DNA molecule are indicated by the DOS calculated at each electronic energy using Green's function [17].

$$G(k, z) = \frac{1}{(z - \text{Im} \eta)[I] - H(k) - \sum(k)} \quad (3)$$

In equation (3), the variable  $z$  represents energy of an electron that travels across the DNA molecule. Symbol  $\text{Im}$  and  $\eta$  respectively represent the imaginary part and an infinitesimal number. The identity matrix is represented by  $[I]$  and the Hamiltonian in matrix form is represented by  $H(\vec{k})$ . The variable  $\sum \vec{k}$  represents the correction on electron Green's function in the poly(dA)-poly(dT) DNA molecule due to the left and right electrodes.



**Figure 3.** Density of states vs energy for poly(dA)-poly(dT) DNA with twisting-motion frequency 0.51 meV at zero temperature and several magnetic field strengths (a) 0 T, (b) 1.231 T, (c) 5.321 T, and (d) 7.356 T.

### 3. Results and discussion

Figure 2 shows DOS spectra with zero external magnetic field, twisting-motion frequency 0.51 meV, and at a selection of temperatures. At 0 K (figure 2a), the DOS spectrum shows three ranges of electron energies at which DOS value is zero: 7.0–7.6 eV, 7.9–8.3 eV and 9.25–9.3 eV. This means that no electrons can occupy these energy levels. As temperature increases, the overall DOS values decrease but the band gaps narrow (figure 2b, figure 2c and figure 2d). At 0 K, the maximum DOS value is over 1000. When the temperature is 77.2 K the maximum DOS value is around 600. Nonzero temperatures cause phonons to appear in the DNA structure, which affect the charge-transport mechanisms. These phonons widen the distribution of twisting angles between A and T bases, introducing disorder to the DNA structure. Therefore, as the temperature increases, the DOS tends to decrease, but the gaps in the DOS spectra narrow. Next, at temperatures far from absolute zero, similar to conductor materials, electrons can occupy every energy level in poly(dA)-poly(dT) DNA molecules. However, at these temperatures, these states are localized [15]; thus, the molecule behaves as an insulator.

DOS spectra at zero temperature, twisting-motion frequency 0.51 meV, and a selection of magnetic field strengths are shown in figure 3. The width of the band gaps in the allowed energy levels remains constant as magnetic field strength increases in figure 3b, figure 3c and figure 3d. These gaps form because of the electron structure of the three nucleotides that make up the poly(dA)-poly(dT) DNA molecule, which are adenine, thymine, and backbone. The presence of a magnetic field increases the peak DOS values, and a higher value means that electrons are more likely to occupy the energy level. This characteristic is caused by the modification of complex hopping amplitudes by the Peierl transition, which changes the value of inter-base hopping amplitude along the molecule with

increasing external magnetic field. This disorder in the electron-hopping amplitude along the molecule structure reduces the freedom of electrons with certain energies to move among the sites on the DNA molecule.

#### 4. Conclusions

The results of the calculation of DOS versus energy have been succeeded in showing the influence of effects of external magnetic field and temperature on the charge-transport properties of poly(dA)-poly(dT) DNA. An external magnetic field modifies the electron-hopping integral of the DNA molecule and can be represented with the Peirels phase factor. This modification affects charge transport as the strength of the magnetic field increases, so the peak values of DOS increase as magnetic field increases and electrons tend to occupy certain sites on the DNA molecule. The gaps in the DOS spectra become narrower as the temperature increases at the expense of lower DOS value. Since all available energy states are localized states at temperatures much above absolute zero, the molecule behaves as an insulator.

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