MAGNETIC FIELD, TEMPERATURE, AND SPIN-POLARIZATION EFFECTS ON ELECTRON TRANSPORT THROUGH DNA MOLECULES

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To my family
ABSTRACT

The deoxyribonucleic acid (DNA) has been widely recognized as the hereditary material found in all organisms. It consists of four nucleotide bases adenine (A), guanine (G), cytosine (C), and thymine (T) linked to a sugar-phosphate backbone. The hydrogen bonds, together with the base-pairs rules of the nucleotide bases, form the double-stranded DNA strand. This thesis aims to study the theoretical analysis of the electron transmission through a two-dimensional, four-channel DNA model, specifically the effect of the magnetic field, temperature, and electron spin. It also includes the graphical outputs on the transmission, 2-D and 3-D contour plots, Lyapunov coefficient, localization length, current-voltage characteristics, spin polarization, and spin-polarized current. Due to the presence of magnetic flux on DNA, the Aharonov-Bohm oscillation with the periodicity of AB oscillations in the transmission and a semiconductor behavior in I-V characteristics could be observed. The increase in temperature can reduce the electron transmission and conductance of the DNA regardless of its sequencing (i.e. periodic, mismatched, or palindromic). However, the highest current could be found in a periodic DNA sequence. The research findings also show that the double-stranded DNA serves as a perfect spin filter despite the weak spin-orbit coupling, and therefore its spin filtration efficiency could be enhanced by increasing the DNA length. Depending on the distance between the replacements of the mispairs and the contacts, and to the number of mispairs, the mismatched sequences could affect the spin polarization. The double-stranded DNA could also act as either a semiconductor or a metal depending on the spin-orbit coupling strength, which shows high spin-polarized current. However, the variation on the helix angle only enables double-stranded DNA to serve as a semiconductor with a high percentage of spin-polarized current at a specific bias voltage.
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Chapter 1: Introduction and Overview

Through their joint effort in 1950s, biologist James Watson and physicist Francis Crick unraveled the double helix structure of deoxyribonucleic acid, commonly known as DNA [1]. According to them, such structure could generally be described as the twisted formation of two DNA strands. As exhibited in Fig. 1.1(a), each DNA strand in a double helix structure contains nucleotides formed through the alternating series of deoxyribose sugar group and phosphate group. Each deoxyribose sugar connects to one of the nucleotide bases namely, guanine (G), adenine (A), cytosine (C), and thymine (T). In a double helix structure, the nucleotides, regarded as DNA strand’s backbone, could be found in a DNA strand’s outer portion while the nucleotide bases are situated in the inner portion. A double helix structure connects two nucleotide strands by hydrogen bonds. However, not all combinations of nucleotide bases can be considered as valid. The principle of nucleotide pairing base indicate that G could only be linked with C, while A could only be linked to T [2].

Similar to a spiral staircase, a double helix structure presents DNA strands in a twisted figure as shown in Fig. 1.1(b). In these strands, DNA molecules run in the opposite direction – an occurrence is often referred to as anti-parallel [1]. To make one full turn in its axis, it takes 10 base-pairs with 3.4 nm for each turn. A double helix DNA structure has a diameter of 2 nm and a vertical distance of 0.34 nm between each base-pair. Traditionally, DNA has been known for its coding function conveyed through genetic and hereditary data. However, in recent years, DNA has been discovered to possess the ability to carry electric current charge through its strands; thus, sparking the interests of numerous scientists from various scientific fields, ranging from chemistry
to nanotechnology, to know and study more about the components and characteristics of a DNA molecule [3, 4].

![DNA Structure](image)

**Fig. 1.1.** (a) A closer look at the DNA structure with alternating series of deoxyribose sugar and phosphate groups, and its nucleotide bases. (b) DNA strands in a double helix structure contain various components with corresponding measurements. ([www2.nau.edu/lrm22/lessons/dna_notes/dna_notes.html](http://www2.nau.edu/lrm22/lessons/dna_notes/dna_notes.html))

Through the aid of technological breakthroughs, the theoretical and experimental methods in studying the fundamental properties of a DNA molecule have greatly improved, which enables scientists to present new insights on this field [4]. In line with their long and continuous search for the most efficient material that could work well with silicon, which is considered relevant among computer factories [5], researchers have been considering the application of DNA molecules in nanotechnology. Due to its stacked structure base-pairs, DNA could serve as one of the appropriate materials in designing new electronic circuits as researchers hope to overcome the limitations in using traditional silicon for electronics [3]. Also, this facilitated the way to the discovery that DNA possesses natural identifying characteristics such as self-assembling, self-recognizing, and self-organizing. Based on these characteristics of DNA, scientists are now considering the probability
of creating an electronic circuit using solely DNA. Its self-recognizing and self-organizing traits would allow the DNA to identify other strands with the same components and connect with them; hence letting DNA produce its own self-assembling biological wire that could be utilized for electrical conduction [6]. Such self-assembled wire structures could be controlled by modifying its base sequence, which presents great potential in developing nano-templates and nano-machines. It could also serve as a nano-electronic material for biological wires [7] and aid in the creation of functional circuits [8].

Aside from DNA’s ability to carry the electric current charge, another aspect that sparked scientists’ interests would include the possibility that DNA could also transport electrons. Research shows that DNA also has the ability to alter its material properties; thus, enabling it to act as a metal [7], semiconductor [7,10], superconductor [9], conductor [10], or insulator [7, 9], depending on the environmental conditions that researchers would use. These environmental conditions include alteration in base sequences and application of water connected to the DNA [7].

Past research reveals that electron conductivity varies depending on the distance between the donor and the acceptor. The wider the distance, the weaker the conductivity level is [9, 11]. However, in research made by Fink and Schönenberger, electron conductivity changes based on the amount of the applied electric current to DNA molecules in a single rope with at least 600 nm long. Based on the $I-V$ curve behavior, as exhibited in Fig. 1.2, the experiment shows efficient electron conduction despite the long distance. Surprisingly, they said $I-V$ curve presents a similar behavior when conducting through polymer; thus, making polymer an excellent semiconductor. Given such results, the researchers found that DNA would be the perfect addition in creating mesoscopic electronic devices [11]. Aside from this, the double helix DNA structure could also be utilized for thermally driven charge transport purposes depending on the dielectric constant [12].
Fig. 1.2. *I-V* behavior of DNA molecules in a 600 nm long single rope indicates an efficient conduction [11].

In a research made by Porath *et al.* [10], the electron transmission was measured through 30 base-pairs (10 nm long) in double-stranded poly(G)-poly(C) DNA molecules. As shown in Fig. 1.3, electron transport varies depending on the amount of electric current amperes. The difference could be seen through the behavior of the current-voltage (*I-V*), which could either be above or below the threshold voltage. The electric current increases linearly above the threshold voltage which makes DNA molecules a good conductor. Conversely, the electric current drops to zero below the threshold voltage, which DNA could serve as an insulator. Even if there are some variations on the width of the voltage gap, it would still display a generally similar behavior which is a semiconductor characteristic [10].
Fig. 1.3. The current-voltage (I-V) behavior of 30 base-pairs of double-stranded poly(G)-poly(C) DNA molecules, placed in between two metal nanoelectrodes with a distance of 8nm, shows that DNA could handle the electron transport despite large electric current volts. Though it generally presents the same behavior, some variations exist in terms of voltage gap width, as indicated by the different line colors [10].

To further investigate DNA’s abilities, the researchers measured the conductance of the single DNA in watery solution by placing the DNA duplex between two gold electrodes as shown in Fig. 1.4 [13]. A DNA with poly(G)-poly(C) sequence reveals that an inversely proportional relationship exists between conductance and length. With this, they have resolved that the conductance of a single DNA molecule depends on its length and sequence.
Fig. 1.4. Experimental illustration made by researchers to measure the conductivity of a single DNA molecule when exposed to the aqueous solution. This shows that conductance differs depending on the DNA strand length and its base sequences [13].

Through the discussion of practical experiments, the DNA conductance would largely depend on the experimental environment, nucleotide base sequence, and DNA length. In addition to most experimental research discussed on electron transmission and DNA conductance, theoretical research by Li and Yan studied electron transport through a DNA molecule with a length of 10 nm (30 base-pairs) as displayed in Fig. 1.5. Consistent with the study made by Porath et al. [10], this electron transport study clarifies that the current-voltage behavior displays a sharp rise of the current above the threshold voltage [14].
The evaluation of the current-voltage characteristics in the DNA system can be found after calculating the electron transmission. Defined as the number of charges passing through a boundary, the voltage applied to DNA molecules dictates the changes on electron conductivity as shown by Fink and Schönenberger [11]. Yoo et al. measured the electron transport through an experimental setup with similar base-pairs of DNA molecules, and further consider gate voltage effect on the current-voltage behaviors. Through this experiment, it detects the probability of creating a DNA field-effect transistor that could function at room temperature with other supplements. Therefore, the measurements of gate voltage dependent transport can demonstrate that the poly(dA)-poly(dT) acts as an n-type semiconductor while poly(dG)-poly(dC) acts a p-type semiconductor. Yoo et al.’s experiment also shows that the varying sequences of DNA base-pairs affect electron transport and current-voltage (I-V) behavior [15]. In the meantime, Wei and Chan discussed and interpreted the I-V results of Porath et al.’s experiment using a tight-binding (TB) model [16]. Their theoretical results were well matched with the experimental data reported by Porath et al. in Fig. 1.6.
Fig. 1.6. Wei and Chan’s theoretical results are well matched with those of Porath *et al.*’s experiment, which confirms that a connection between electrodes and DNA exists where electron transport could be measured through trapped DNA in between electrodes [16].

1.1. Preview

In this paper, we intend to calculate the electron transmission through DNA molecules by taking into account the two-dimensional (2-D) four-channel model of DNA with a double-helix structure of 20 base-pairs connected by electrodes using tight-binding (TB) technique. Due to recent interest in electron-transfer through DNA, we study the magnetic field, temperature, and spin dependent electron transport to gain a better understanding. In Chapter 2, we examine electron transmission through double-stranded DNA in the presence of an external magnetic field with and without backbone effects. We consider different lengths of DNA such as 1 base-pair, 5 base-pairs, and then 20 base-pairs to investigate an Aharonov-Bohm loop interference. We show the periodicity of AB oscillations by changing the value of the applied magnetic field. In Chapter 3, we apply thermal fluctuations into different sequences of 2-D four-channel of DNA in order to investigate the electron transmission, Lyapunov coefficient, and localization length. In Chapter 4, we study the spin-dependent electron transport for different DNA lengths, spin-orbit coupling,
helix angle, and twist angle. We calculate the spin polarization of transmission and show its significance even in case of small spin-orbit coupling (SOC). We also evaluate the spin-polarized current (net spin current) at varying spin-orbit coupling and helix angle. Finally, in Chapter 5, we conclude with the results of our theoretical study and express opportunities for future work.
Chapter 2: The magnetic field effects on electron transmission through a double-strand DNA molecule

2. 1. Introduction

DNA is a genetic material that has interested scientists in many different fields, ranging from biology to nanoscience. Over 60 years ago, the historic paper on the structure of DNA was published [17]. Since then, a number of experimental and theoretical investigations have been done to study the electron transport through dry and wet DNA molecules. Some previous investigations studied electron transmission through single-stranded DNA, while others studied double-stranded (ds) DNA. In a 1-D system, the fishbone model, which ignores the hydrogen bonds between the bases, was used. However, in 2-D system, the ladder model was used, which represents the hydrogen bonds between the bases and the sugar-phosphate backbones in the DNA structure [18].

In addition, different experiments have been done to observe the effects of different factors, such as a magnetic field, on electron transmission. In the medical field, a group of researchers studied the effects of the exposure of human cells to an electric or magnetic field [19, 20]. In the physics field, some researchers examined the effects of magnetic flux on electron transport through a linear array of nanoscopic rings [21, 22].

In this chapter, we focus on studying the electronic properties of DNA molecules with the existence of an external magnetic field. Yi et al. studied the electric properties of DNA molecules with hairpin-like shapes in the presence of magnetic flux. They found that the current oscillated when the flux changed [23]. Wong et al. have also investigated the effect of an external magnetic field on DNA electronic conductivity by examining the efficiencies of photoinduced DNA-mediated charge transport (CT) through guanine damage, as shown in Fig. 2.1. They found positive
enhancements in the decomposition of 8-cyclopropyl deoxyguanosine \((_{8\text{CP}}G)\) at the proximal and distal guanine doublets after applying a static magnetic field of 300 mT. They concluded that the electronic conductivity of duplex DNA can be enhanced by applying an external magnetic field [24]. Motivated by these results, we expose a closed loop of DNA to an external magnetic field and find the Aharonov-Bohm (AB) effect. The AB effect is a phenomenon that describes the interaction between charged particles, DNA in our case, and magnetic fields in space. When a beam of electrons moves toward a solenoid, it splits in two and sends each beam to a different side. After that, the electron beams combine on the other side of the solenoid by a factor proportional to the enclosed flux. Our purpose is to study the effect of the magnetic field on double-helix DNA to understand the possible conduction in order to use DNA in electronic components. That means that the application of magnetic flux through the DNA serves as a parameter of interest in its effect on electron transmission.

![Diagram of DNA-mediated CT in the presence of an external magnetic field](image)

Fig. 2.1. The experimental design of DNA-mediated CT in the presence of an external magnetic field [24].
2. 2. Two-dimensional four-channel of the DNA structure using tight-binding model

To gauge the electron transmission through the DNA molecule, the 2-D four-channel model of the DNA structure is employed in this study. Close monitoring shows that electron transmission and current through the DNA molecule varies depending on the experimental environment and the applied voltage. Generally, the structure of this model comprises of bases – guanine (G), adenine (A), cytosine (C), and thymine (T) – which could serve as conduction channels for electron transmission. A 2-D four-channel model could only be materialized by integrating hydrogen bonds, intra-backbone couplings, and coupling between DNA base-pairs and backbone. Linked between two semi-infinite electrodes, the electron transmission in a DNA molecule can be manifested through four channels comprised of π-orbital that intersects with the main conduction chains’ neighboring bases and the upper and lower backbones of the DNA, as depicted in Fig. 2.2.

Fig. 2.2. 2-D four-channel model of DNA with two contact leads: $\varepsilon_0 = 7.75$ eV (lead onsite energy), $e_i$ (i = 1-40 nucleotide base onsite energy), and $e_a = 8.5$ eV (backbone onsite energy). Dashed lines represent hopping amplitudes: $V_0 = 1$ eV (inter-lead coupling), $h_i$ (i = 1-20 hydrogen bonds), $B_a$ (backbone-to-backbone coupling), $t_{i,i+1}$, $T_{i,i+1}$ (intra-chain of nearest-neighboring bases), $V_{L1,L2}$, $V_{R1,R2}$ (coupling between the end bases and leads), and $V_a$ (coupling between the DNA bases and the backbones).
Figure 2.2 illustrates a 20 poly(G)-poly(C) or poly(A)-poly(T) base-pair DNA model, where the circles in the middle represent the DNA nucleotide bases, the hexagons in the upper and lower portions for the sugar and phosphate backbone groups, and the alienated circles on each side as lead sites. These elements are connected through the dashed lines, which represent the hopping amplitude between the base-pair themselves ($t_{i,i+1}$, $T_{i,i+1}$), between the base-pairs and the backbone ($V_a$), and between the end bases and leads ($V_{L1,L2}$, $V_{R1,R2}$) in a horizontal and vertical direction. Furthermore, the hopping amplitudes, $B_a$ and $V_0$, interconnects backbones and the leads, respectively, while hydrogen bonds ($h_i$) interlink each base-pair which has onsite energy $e_i$ ($i = 1$-40 for nucleotide bases). It should also be noted that each nucleotide carries an onsite energy based on ionization potential of each base, $G = 7.75$ eV, $C = 8.87$ eV, $A = 8.24$ eV, $T = 9.14$ eV, and $8.5$ eV for backbones.

With this, the TB Schrödinger equation is written as:

$$-\sum t_{n,m} \psi_m + e_n \psi_n = E \psi_n, \quad (2.1)$$

where the matrix elements, $t_{n,m}$, are couplings between $n$ and $m$ sites. The total Hamiltonian of the system can be written:

$$H_{Tot} = H_{Leads} + H_{DNA} + H_{Leads-DNA}. \quad (2.2)$$

Here, the total Hamiltonain can be described by the three parts: the DNA structure, the leads themselves, and the coupling between the end of the DNA and the leads. The Hamiltonian for the leads themselves is:

$$H_{Leads} = \varepsilon_0 \sum_i l_i^* l_i - V_0 \sum_i (l_i^* l_{i+1} + h. c). \quad (2.3)$$

The Hamiltonian for a DNA molecule is:
where $c_i^* (c_i)$, $d_i^* (d_i)$, $a_i^* (a_i)$ and $b_i^* (b_i)$ are the creation (annihilation) operators at $i$-th base and $e_i$ and $e_j$ are the onsite potential energy of the DNA. The DNA molecule is coupled to two semi-infinite metallic leads by the tunneling Hamiltonian:

$$H_{Leads-DNA} = -V_{L1} l_i^* c_1 - V_{L2} l_i^* d_1 - V_{R1} l_i^* c_N - V_{R2} l_i^* d_N + h.c.,$$  

(2.5)

where $V_{L1(2)} (V_{R1(2)})$ are the hopping strengths between the left (right) lead and the end DNA bases, and $l_i^* (l_i)$ is the creation (annihilation) operator at the $i$-th site of the leads.

The general incoming and outgoing wave functions in the leads can be written as:

$$\psi_n = e^{i n \theta} + r e^{-i n \theta} \quad (n \leq 0),$$

$$\psi_n = t e^{i n \theta} \quad (n \geq 1),$$  

(2.6)

here, $\theta = k \alpha$, where $\alpha$ is lattice constant, which is the distance between nearest-neighbors and $k$ is the wave vector that is connected with the energy by the dispersion relation for the Bloch states, $E = -2 t_0 \cos k \alpha + e_0$, $r$ is the reflection amplitude, and $t$ is the transmission amplitude [25-26].

The Schrödinger equation of the tight-binding (TB) model uses a total of 82 site wave functions which consist of 2 lead sites, 40 sugar-phosphate backbones, and 40 bases including G, C, A, or T. By applying these wave functions into the TB Hamiltonian equation, an $82 \times 82$ matrix can be obtained. By solving the matrix equation for the linearized TB Hamiltonian, we obtain the transmission amplitude as a function of the incoming energy, $t(E)$. Similarly, the transmission coefficient is obtained by squaring the transmission amplitude [27, 28].
\[ T = |t(E)|^2. \]  

(2.7)

Since the transmission function is directly related to the current, the \( I-V \) characteristics obtained from the Landauer–Büttiker formula at room temperature [28-32] can be written as:

\[
I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E) \left[ f_L(E) - f_R(E) \right] dE. 
\]  

(2.8)

Here, \( f(E) \) is the Fermi-Dirac distribution, \( f_L(R)(E) = \frac{1}{e^{\beta[E-\mu_{L(R)}]} + 1} \), where \( \beta = \frac{1}{k_B T} \) and \( \mu_{L(R)} \) represents the leads’ electrochemical potential which depends on the applied bias voltage. We choose the leads’ electrochemical potential as \( \mu_L = E_f + (1 - \eta) eV_{sd} \) and \( \mu_R = E_f - \eta eV_{sd} \), where \( V_{sd} \) stands for source-drain applied voltage, \( E_f \) stands for equilibrium Fermi energy, and \( \eta \) is a parameter denoting the probability of contact to leads asymmetry (\( \eta = 0.5 \)) [28-32]. The \( I-V \) characteristics vary based on the relative values of the Fermi energy because the Fermi energy window mainly contributes to the conduction.

In this chapter, we analyze the electron transport properties of homogeneous DNA in the presence of an external magnetic field. We use the tight-binding (TB) model to calculate the electron transmission. A magnetic field penetrating at the center of a 2-D DNA structure of 20 base-pairs produced an AB phase difference between the electron wave functions of the upper and lower DNA strands in the absence and presence of backbone effects. To examine quantum interference through the 2-D DNA structure, we multiply the hopping amplitude between the upper and lower DNA strands, coupling between leads and DNA, and the interconnected backbones by a phase factor as follows:

\[
t(T)_{l,i+1} \rightarrow t(T)_{l,i+1} e^{\pm i\phi}, B_a \rightarrow B_a e^{\pm i\phi}, V_{Leads} \rightarrow V_{Leads} e^{\pm i\phi}. 
\]  

(2.9)
The total phase shift is \( \phi = 2\pi \Phi / (M\Phi_0) \), where \( \Phi \) is the magnetic flux through the double helix DNA in units of flux quantum \( (\Phi_0 = h/e) \) at even-number sites or \( (\Phi_0/2) \) at odd-number sites [33, 34]. Here, \( M \) is the total number of sites, including two sites of semi-infinite electrodes. In our system, \( M \) is 42 without considering the backbone effects (20 for G bases, 20 for C bases, and 2 lead sites) and becomes 82 with the backbone effects (20 for G bases, 20 for C bases, 20 for upper backbones, 20 for bottom backbones, and 2 lead sites). The minus sign in a phase factor of Eq. (2.9) indicates that the electron moves in a clockwise direction, while the plus sign indicates that the electron moves in a counterclockwise direction. We also examine the electron transmission and conductivity through DNA molecules under the effect of the magnetic field variation.

### 2.3. Magnetic field effects on the DNA molecule in the absence and presence of backbone effects

Some researchers have studied the electron transmission through the DNA structure in the absence of backbone effects, while others have observed the electron transmission through the double helix structure of DNA. Guo et al. reported the effects of backbone disorder on the properties of the electron transmission of biological and synthetic DNA molecules [35]. They observed this effect by varying the backbone disorder degree and found out that the duplex DNA showed poor transmission as the backbone disorder degree increased. However, as the environment-induced disorder surpasses a critical value that gives rise to a semiconducting-metallic transition, the charge transport ability of DNA molecules increases. Macia et al. have observed the major role of backbone-induced effects in electron transmission through ploy(G)-poly(C) and poly(A)-poly(T) chains [36]. They introduced a two-step renormalization process for the energy spectrum and transmission coefficient to describe ds-DNA in terms of an effective
single channel. In addition, they described the significant changes in electron transmission as well as $I$-$V$ features. Cuniberti et al. have studied charge transport through identical poly(G)-poly(C) ds-DNA molecules in the presence of the backbone effects [37]. They observed that backbone coupling, which is the hybridization of the overlapping $\pi$ orbitals in the base-pair with the backbone, could control the existence of a gap in the transmission and change the $I$-$V$ characteristics.

Since backbone coupling plays an important role in transmission, we first investigate the electron transmission of 20 poly(G)-poly(C) DNA molecules with and without backbone effects in the presence of a magnetic field as shown in Fig. 2.3(a) and (b). Here, DNA molecules may have a single ring or multi-rings, which are connected to semi-infinite electrodes from the left and right sides and are linked by the hopping amplitude between adjacent bases, depending on the existence of hydrogen bonds between bases. Second, we study the effects of variation in the hydrogen bonds between base-pairs and the coupling between leads and DNA in electron transmission through DNA in the presence of an external magnetic field.
Fig. 2.3. 2-D four-channel TB model of electron transport in the presence of a magnetic field when (a) neglecting backbone effects and (b) taking into account backbone effects.

2.3.1. Variation of the hydrogen bonds

Hydrogen bonding has a significant role in electron transport through DNA [38, 39]. Hydrogen bonds in DNA base-pairs are the best-known example, which improves the stability of DNA base-pairs and holds the chains of DNA (G with C or A with T) together. Jauregui et al. have studied the electronic differences between ds-DNA nucleotides in order to understand the type and
sequence of ds-DNA nucleotides [40]. They found very poor discrimination between ds-DNA nucleotides due to the lower conductivity in the DNA backbone region. Moreover, they noticed the electrical characteristic is not just natural in the ds-DNA nucleotides, but it also depends on the presence of counterions in the system.

In order to see the effects of hydrogen bonds variation \( (h_i) \), we select different numbers of poly(G)-poly(C) base-pairs (one base-pair, 5 base-pairs, and 20 base-pairs) of ds-DNA molecules and study the AB effect on electron transmission through these systems. We fix the parameters \( V_{Leads} = 0.3 \text{ eV} \) (a hopping amplitude between leads and end bases), \( t(T)_{i,i+1} = 0.2 \text{ eV} \) (intra-chain of the nearest neighbor bases), \( \varepsilon_0 = 7.75 \text{ eV} \) (lead onsite energy), and \( V_0 = 1 \text{ eV} \) (intra-lead coupling). We calculate the transmission and contour plots of the transmission as a function of the magnetic flux for each case.

Fig. 2.4. A single base-pair DNA molecule is linked by two contact leads in the presence of the AB effect with the (a) negligence of the backbone effect and (b) existence of the backbone effect.

We first consider a single base-pair DNA structure in the absence and presence of backbone effects in Fig. 2.4. The existence of the hydrogen bond between base-pairs \( (h_i \neq 0) \) can cause a
change in the number of loops in the DNA structure (from red to green loops). The transmission characteristics for different values of the hydrogen bond are studied to see AB interference of this structure. Figure 2.5 shows the transmission and contour plots of the transmission as a function of the magnetic field without and with backbone effects for three different values of hydrogen bonds [$h_i = 0, 0.3, \text{and } 0.5$ (left to right)] at a fixed incoming energy $E = 8$ eV. In the absence of backbone effects, shown in Fig. 2.5(a), we find that the periodicity of the AB oscillations is $1\Phi_0$ (one red loop) at $h_i = 0$, but the periodicity of the AB oscillations is $2\Phi_0$ (two green loops) at $h_i \neq 0$. As expected, the periodicity increases as the number of loops increases. It also causes a change in the form of the oscillation, where the peak is split into two equal peaks. In the presence of backbone effects, shown in Fig. 2.5(b), the periodicity in the transmission changes from $1.5\Phi_0$ at $h_i = 0$ to $3\Phi_0$ at $h_i \neq 0$. 
Fig. 2.5. The flux dependence of transmission at fixed incoming energy \((E = 8.0 \text{ eV})\) and contour plots of the transmission vs magnetic flux and electron energy for different values of hydrogen bond \(h_i\) (a) without the backbone effects and (b) with the backbone effects.

Next, we consider five base-pairs of poly(G)-poly(C) ds-DNA in the absence and presence of backbone effects in Fig. 2.6. Flux dependence on the transmission and contour plots of the transmission as a function of flux and electron energy are shown in Fig. 2.7. At \(h_i = 0\), the amplitude of oscillations in the transmission is so small due to small AB interference, which is shown in the inset of Fig. 2.7. Increasing the value of hydrogen bonds from \(h_i = 0 \text{ eV}\) to 0.4 eV
leads to the clear emergence of oscillations in the transmission. In the absence of backbone effects shown in Fig. 2.7(a), the periodicity becomes $6\Phi_0$ and the transmission at the zero flux is maximal. However, in the presence of backbone effects in Fig. 2.7(b), the periodicity becomes $11\Phi_0$ due to the increase of the number of loops in the DNA structure and the electron transmission at the zero flux is minimal.

Fig. 2.6. Sketch of five poly(G)-poly(C) base-pairs under the effect of the magnetic field in the (a) absence of backbone effects and (b) presence of backbone effects.
Fig. 2.7. Flux dependence on the transmission and contour plots of the transmission vs flux and electron energy, showing AB oscillations for \( h_i = 0 \) and \( h_i \neq 0 \) in the (a) absence of backbone effects at \( E = 8.0 \) eV and (b) presence of backbone effects at \( E = 9.0 \) eV.

Finally, we consider 20 poly(G)-poly(C) base-pairs ds-DNA for \( h_i \neq 0 \) in the absence and presence of backbone effects to observe the AB oscillations in Fig. 2.8. We note that increasing the number of base-pair leads to an increase in the number of loops in the DNA structure. Hence, we expect a direct proportional relationship between the periodicity of AB oscillations and the number of loops in DNA [41].
Fig. 2.8. Structure for twenty base-pairs of poly(G)-poly(C) ds-DNA under the magnetic field effects in the (a) absence of backbone effects and (b) presence of backbone effects.

In Fig. 2.9, we present contour plots of the transmission vs a magnetic flux and $h_i$ with $E = 9.0$ eV and the transmission $T(E)$ vs a magnetic flux at $h_i = 0.1, 0.2, 0.3, 0.4,$ and $0.5$ eV in the absence and presence of backbone effects. We find the periodicity of the AB oscillations in the presence of backbone effects becomes double the periodicity in the absence of backbone effects. It is seen that the shape and the amplitude of the oscillations in the transmission change as the value of $h_i$ changes. At $h_i = 0.1$ eV, the electron transmission in the presence of backbone effects is much higher than that in the absence of backbone effects. From Fig. 2.9(a) and (c), we clearly
see an oscillatory feature in the transmission as a function of $h_i$ for a fixed magnetic flux, especially in the range of $h_i > 0.2$.

Fig. 2.9. Contour plots of the transmission vs a magnetic flux and $h_i$ with $E = 9.0$ eV: (a) without backbone effects and (c) with backbone effects. $T(E)$ vs a magnetic flux for $h_i = 0.1$ eV (blue line), 0.2 eV (green line), 0.3 eV (purple line), 0.4 eV (orange line), and 0.5 eV (gray line): (b) without backbone effects and (d) with backbone effects.
2.3.2. Variation of contact coupling between leads and DNA

It is a challenge to connect DNA molecules to electrodes in most experimental measurements. Researchers reported in some experiments that connecting DNA molecules to electrodes required laying the DNA molecules directly onto the electrodes. They used various electrodes in their experimental measurements, such as gold electrodes [42], metallic electrodes [43], and graphene electrodes [44]. In order specifically to address DNA-lead contact effects on charge transport, we use a theoretical approach to examine the effect of contact coupling between leads and DNA in the presence of an external magnetic field.

We calculate the electron transmission through twenty base-pairs of poly(G)-poly(C) DNA by varying the coupling strengths symmetrically in the presence of an external magnetic field. In Fig. 2.10, we show the transmission vs $\Phi/\Phi_0$ for different values of $V_{Leads} = 0.3, 0.5,$ and $0.7$ eV and contour plots of transmission as a function of $\Phi/\Phi_0$ and $V_{Leads}$ at fixed incoming energy $E = 9.0$ eV and $h_l = 0.5$ eV. We note that the change in the incoming (outgoing) coupling strength does not affect the periodicity of AB oscillations in the electron transmission for both the absence and presence of backbone effects. In the weak coupling regime for both the absence and presence of backbone effects, $V_{Leads} = 0.3$ eV, the transmission at $\frac{\Phi}{\Phi_0} = 10$ has a maximal value and the electron tunneling between DNA and leads increases. On the other hand, in the strong coupling regime for both the absence and presence of backbone effects, $V_{Leads} = 0.7$ eV, the transmission at $\frac{\Phi}{\Phi_0} = 10$ reaches to a minimal value and the electron tunneling between DNA and leads decreases. Notice that increasing the value of $V_{Leads}$ leads to decrease the electron transmission for a fixed flux, $\frac{\Phi}{\Phi_0} = 10$. 
Fig. 2.10. Contour plots of the transmission vs a magnetic flux and $V_{\text{Leads}}$: (a) without backbone effects and (c) with backbone effects. T(E) vs a magnetic flux for various values of symmetric coupling strength: (b) without backbone effects and (d) with backbone effects.
2.3.3. Variation of magnetic flux

Magnetic flux is the number of magnetic field lines that exert force on a moving charged particle or on other magnetic material. Bayer et al. have exposed a charged particle moving in a nano-size semiconductor quantum ring subjected to a perpendicular magnetic field. They observed Aharonov-Bohm (AB) oscillations in the emission of a charge in the single ring structure [45]. Hedin et al. studied the transmission of electrons through a connected multi-ring system in the presence of an external magnetic field [21]. They changed the applied magnetic flux to study the magnetic field effects on electron transmission.

In this section, we analyze the effects of modulating magnetic flux on DNA transmission and conductivity with and without backbone effects. We plot the transmission as a function of energy for different magnetic flux value in the absence and presence of backbone effects and contour plot of the transmission as a function of a magnetic flux and electron energy in Fig. 2.11. We fix parameters as $V_{\text{Leads}} = 0.3$, $t(T)_{i,i+1} = 0.2$, $\varepsilon_0 = 7.75$, $\hbar = 0.1$, $V_a = 0.1$, and $V_0 = 1$ in units of eV. The horizontal dashed lines for a magnetic flux in the contour plot indicate the periodicity of AB oscillations in the electron transmission. We first examine the DNA transmission without an external magnetic flux ($\Phi/\Phi_0 = 0$) for both with and without backbone effects. In both cases, the transmission has two minibands with a gap. In the presence of backbone effects, however, extra resonant peaks arise within the transmission gap and an overlap of these peaks with second miniband occurs when the incoming electron energy has close to the value of the energy level of the backbone. In the absence of the backbone effects, we observe that the transmission are the same at $\Phi/\Phi_0 = 0$ and 21 or $\Phi/\Phi_0 = 10$ and 31, which indicates that the periodicity of AB oscillations is 21 $\Phi/\Phi_0$. In the presence of the backbone effects, we plot $T(E)$ vs $E$ for $\Phi/\Phi_0 = 0$ and 21.
0, 20, 41, and 61, respectively. We see the same transmission at \( \frac{\Phi}{\Phi_0} = 0 \) and 41 or \( \frac{\Phi}{\Phi_0} = 20 \) and 61.

Fig. 2.11. Contour plots of the transmission as a function of energy and a magnetic flux (a) without backbone effects and (c) with backbone effects. Transmission as a function of energy for different magnetic flux (b) without backbone effects and (d) with backbone effects.
In order to understand more about the properties of electron transmission through DNA in the presence of an external magnetic field, we calculate the $I$-$V$ characteristics, using Eq. (2.8) with $E_f = 6.3\, \text{eV}$ and $T = 300\, \text{K}$ at different values of magnetic flux as shown in Fig. 2.12. The existence of the gap in the $I$-$V$ curves indicates a semiconductor-like behavior in both cases. We find the $I$-$V$ curves are identical for $\frac{\Phi}{\Phi_0} = 0$ and 21 without backbone effects. In the presence of backbone effects, the $I$-$V$ curves are the same for $\frac{\Phi}{\Phi_0} = 0$ and 41. As expected, the $I$-$V$ curves are also affected by the periodicity of AB oscillations.

Fig. 2.12. Current as a function of the source-drain applied voltage for different magnetic flux (a) without and (b) with backbone effects. We plot each I-V curve separately as shown in the insets.
Chapter 3: Temperature effects on ds-DNA molecules

3.1. Introduction

Electron transport through deoxyribonucleic acid (DNA) molecules is a very interesting topic for study. Recently, the attention of chemists and physicists has been drawn to the possible employment of DNA in molecular electronics. They found that DNA could act as a rectifier, transistor, switch, or wire depending on the electronic property configuration [46, 47, 48]. Crick and Watson established the chemical formula of DNA, a series of chained molecules created by connecting multiple complex monomeric units called nucleotides. The four nucleotide types are guanine (G), adenine (A), cytosine (C), and thymine (T). They can vary in number and differ in sequence, depending on the chain and on the species [49]. The base pairing relationship of the DNA molecules, selectively established as A–T and C–G pairs attached by hydrogen bonds, represents the genetic information stored in the DNA; the pairs are held in the double-helix structure by a sugar-phosphate backbone [50]. Despite some ambiguity associated with DNA’s chemical and physical properties, many scientists use the fundamental knowledge to explore the formation of DNA structure and its influencing factors [51]. However, very few attempts have been made to study the thermal and thermodynamic properties of DNA. One such attempt was made by Meyer et al., who studied extensive molecular dynamics simulations of different sequences of DNA at five different temperatures, ranging from $273 \, K$ to $350 \, K$ [52]. They found that the effect of temperature in each sequence showed as a regular linear decrease in stiffness. Similarly, Rahman and Yudiarsah investigated the temperature effect on the charge transport properties of G-quadruplex (G4) DNA molecules [53]. They found that the temperature effect leads to disorder in these molecules and to a decrease in electron localization length. Moreover,
Chand has observed the current-voltage of an inhomogeneous Schottky diode based on a Gaussian distribution, finding that, at very low temperatures, Schottky diodes show higher currents than at higher temperatures [54].

Focusing on DNA structure, biochemistry scientists have used DNA tiles to build blocks for producing DNA nanostructures, linking them with branched junctions called sticky-end DNA [55, 56, 57]. They use self-assembling nanostructures to create a two- or three-dimensional DNA structure by mixing short single strand of the DNA. Specifically, Seeman discovered ways to connect DNA molecules by sticky ends and produced long lines, cyclic order, rotary or scaffold structures as specific components for one or two dimensions of DNA molecules [58].

![Fig. 3.1](image)

Fig. 3.1. (a) Four DNA strands bound together to form four double-helical arms, (b) DNA double crossover units, (c) Rotary DNA nanomachine, and (d) DNA scaffolds used to organize boxes into crystals [58].

To gain a deeper understanding of DNA sequencing, Bell et al. determined the first partial DNA sequence information directly using an electron microscope. They used atomic-resolution imaging of specific sequences and heavy atoms labeled in short DNA molecules as shown in Fig.3.2. [59].
In bionanomaterial area, researchers have used a tight-binding formulation to study the nucleotide correlations and electronic transport of single-strand DNA segments [60]. They used either a Rudin-Shapiro quasiperiodic sequence (RS) with a long-range pair correlation or a random sequence (PC) with a short-range pair correlation, comparing each sequence to the first sequenced human chromosome 22 (Ch22). They found that the amplitudes of RS sequences are regularly larger than Ch22 and PC sequences. They also examined the transmission and Lyapunov coefficient as a function of energy for Ch22 and RS sequences with varying numbers of nucleotides.

In this chapter, we study thermal properties of double-stranded DNA and electron transport due to the temperature effects. Specially, we focus on how different DNA sequences in the presence of thermal fluctuations affect the transmission properties. To study electron transmission and I-V characteristics produced by temperature variations in our system, we consider three different sequences such as periodic, mismatched, and palindromic sequences. In order to examine
transmission properties of these different sequences, the Lyapunov coefficient and localization length are calculated.

3. 2. Methodology

We consider the double-strand DNA model, as it can represent the actual design of the DNA more accurately. Figure 3.3 shows a diagram of a ds-DNA molecule with 20 base-pairs of A, T, G, and C nucleotides and with applied thermal fluctuations. The DNA bases G, C, A, and T are given by the ionization potentials, taken as 7.75, 8.87, 8.24 and 9.14 eV, respectively. Since variation of the temperature induces the structural disorder and fluctuations of the system, it is important to investigate the transport behavior for electrons through DNA by applying temperature-dependent hopping strengths. Hence, we apply the variation of the temperature into the hopping integrals in terms of twist-angle fluctuations.

Fig. 3.3. A schematic of four-channel, 20 base-pairs of ds-DNA under the thermal fluctuation effects. The DNA structure is destabilized by increasing temperature, which creates structural disorder on the hopping integrals.
The twist-angle fluctuations, which affects quantum interference during charge transport, are based on a Gaussian distribution with average twist angle. This average twist angle is 
\[ \langle \theta_{i,i+1} \rangle = 0, \]
where \( \theta_{i,i+1} \) is a relative twist angle deviated from its equilibrium value between 
i and \( i + 1 \). Using the equipartition theorem, \( \langle \theta_{i,i+1}^2 \rangle = \frac{k_BT}{I\Omega^2} \), where \( \frac{I\Omega^2}{k_B} = 250 \ K \), \( \Omega \) is the oscillator frequency, \( I \) is the reduced moment of inertia for relative rotation of two adjacent bases, and \( T \) is temperature [61-64]. This factor enters into our system through the hopping parameter. Hence, we add the variation of temperature \( \cos \theta_{i,i+1} \) into the hopping integrals between the bases, where \( \cos \theta_{i,i+1} \cong 1 - \frac{\theta^2}{2} \cong 1 - \frac{k_BT}{2I\Omega^2} \times X \). The final hopping integrals can be written as

\[
T(t)_{i,i+1} \rightarrow T(t)_{i,i+1} \left[ 1 - \left( \frac{k_BT}{2I\Omega^2} \right) \times X \right]
\]

\[
V_a \rightarrow V_a \left[ 1 - \left( \frac{k_BT}{2I\Omega^2} \right) \times X \right]
\]

\[
h_i \rightarrow h_i \left[ 1 - \left( \frac{k_BT}{2I\Omega^2} \right) \times X \right]
\]

\[
B_a \rightarrow B_a \left[ 1 - \left( \frac{k_BT}{2I\Omega^2} \right) \times X \right],
\]

where \( X \) is a factor giving the random fluctuations such as \( X = 0.5, -0.3, 0.3, -0.5 \).

According to Anderson localization theory, the charge transport under random fluctuation of the twist angle is characterized by a Lyapunov exponent \( \gamma = -\ln \left( \frac{T(E)}{2N} \right) \) and localization length \( \gamma^{-1} \), where \( T \) is the transmission coefficient and \( N \) is the number of bases [64-71]. In our case, we are interested in finding \( \gamma \) and \( \gamma^{-1} \) for different type of DNA sequences that are typically a few tens of base-pair long.
3.3. Temperature effects on a periodic sequence

The charge transport properties of nucleic acids are investigated in order to gain a deep understanding of their biological function and their potential for use in applications such as nanocircuits and nanosensors. Numerous external and internal factors affect carrier motion along DNA molecules [72], base-pair sequence and geometry being two of the internal factors. In this section, we investigate the thermal vibration effects on electron transmission of the periodic poly(G)-poly(C) DNA sequence attached to two semi-infinite leads. We set the parameters in Fig 3.3 as $T(t)_{i,i+1} = 0.2, h_i = 0.3, V_a = 0.3, B_a = 0.1, V_{Leads} = 0.3$, and $V_0 = 1$ in units of eV. The circles in Fig 3.3 denote base-pairs, the light blue spheres are $G = 7.75$ eV, and the purple spheres are $C = 8.87$ eV, while the yellow hexagons represent sugar-phosphate backbone sites with onsite energy $e_a = 8.5$ eV.

In Fig. 3.4, we show the total temperature-dependent transmission coefficient, Lyapunov exponent $\gamma$, and localization lengths $\gamma^{-1}$ as a function of electron energy for three different temperatures. The thermal fluctuations can destroy coherent charge transport and reduce the mean transmission coefficient [73]. It is clearly seen that the transmission bands in the spectra become increasingly fragmented as the temperature rises from 0 K to 300 K. We note that the localization length at $T = 0$ K is larger than that $T \neq 0$ K. However, an increase in temperature reduces the electron transmission and thus makes the electron more localized.
Fig. 3.4. Plots of the transmission, Lyapunov coefficient $\gamma$ and localization lengths $\gamma^{-1}$ as a function of an electron energy for the periodic poly(G)-poly(C) DNA sequence at various temperatures.

In other word, high temperature leads to the disorder of the system and a reduction of the localization length and consequently a reduction of the electron conductance according to the relationship, $T \propto \exp[-L/\xi]$, where $L$ is total length of the system. To clarify the temperature effect on the electron transmission, we also show a contour plot of the transmission as a function of electron energy and temperature. The red dashed lines in Fig 3.5 indicate that an increase of temperature creates more gaps in the transmission through the DNA.
3.4. Temperature effects on a mismatched sequence

Self-recognition of DNA means the four nucleotides connect to each other only through hydrogen-bonded G-C and T-A pairs. However, DNA base-pairs can be exposed to chemical damage, ionizing radiation, or damage from other environmental sources, leading to mispairs within the DNA. The presence of mispairs in the DNA sequence can cause minor changes in the thermodynamic properties and structure of the DNA molecules [74]. Geometric changes in DNA structure occur not only because of mispairs but also because of the altered temperature. Looking at the structural distortion of the DNA induced by mispairs and thermal vibrations, we examine the transport properties of a mismatched sequence of 20 base-pairs DNA. The structure we study is shown in Fig 3.6, in which we replace a canonical G-C base-pairs with an A-A mispairs in the middle of the sequence. The same parameter values mentioned in the previous section are used.

Fig. 3.5. Contour plot of the transmission as a function of energy $E$ and temperature $K$ for periodic poly(G)-poly(C) DNA sequence.
Figure 3.6 shows the temperature-dependent transmission coefficient and the localization length as a function of electron energy. When $T = 0 \, K$, the magnitude of transmission in the first miniband does not reach to a maximum value due to two A–A mispairs in the sequence. Similar to the periodic sequence shown in the previous section, the temperature effects lead to suppression of the resonant peak heights because of increased scattering and fluctuations. The thermal fluctuations make the localization lengths smaller and create more gaps when the temperature increases.
Fig. 3.7. The transmission coefficient (left) and localization length (right) for a mismatched DNA sequence at $T = 0, 100, 200, \text{ and } 300 \, \text{K}$.

In order to see how thermal vibrations affect the electron transmission through DNA, we plot the transmission coefficient $T(E)$ versus a temperature for $E = 7.5, 7.8$, and $9.4 \, \text{eV}$ (see Fig. 3.8). For $E = 7.8 \, \text{eV}$, the maximum transmission is maintained until the temperature reaches $100 \, \text{K}$.
and then the transmission decreases as the temperature increases. For $E = 9.4 \text{ eV}$, the transmission decreases rapidly until $T = 50 \text{ K}$ and the transmission is almost zero when $T > 50 \text{ K}$. For $E = 7.5 \text{ eV}$, the transmission is smoothly depressed when the temperature increases. We conclude that, for any value of Fermi energy, electron transmission through DNA decreases as temperature increases [61].

Fig. 3.8. Transmission vs temperature for different values of incoming electron energy.

3. 5. Temperature effects on a palindromic sequence

DNA sequences play an important role in the human genome function; the palindromic nucleic acid sequence is one of these sequences [75]. The palindromic sequence must be the same when read forward or backward from a central axis of the symmetry. There are two kinds of palindromic DNA sequence; one is exact, with symmetry in the center, while the other is approximate. An exact palindromic DNA sequence is essentially even in length because the middle base of an odd length cannot be the same as its complement [76]. We study electron transmission through an exact palindromic DNA sequence that contains no mismatches in the presence of
thermal vibrations. Figure 3.9 shows the structure of this sequence with nucleotide bases $G = 7.75, C = 8.87, A = 8.24$, and $T = 9.14$ eV.

Fig. 3.9. An exact palindromic sequence of 20 base-pairs DNA.

We set the parameters in our model as $T(t)_{i,i+1} = 0.2$ eV (intra-chain of nearest neighboring bases), $V_a = 0.3$ eV (between the DNA bases and the backbone), $V_{Leads} = 0.4$ eV (between the end bases and leads), $B_a = 0.2$ eV (backbone coupling), $V_0 = 1$ eV (inter-lead coupling), and $h_i = 0.3$ eV (between G-C) and $h_i = 0.2$ eV (between A-T). The plots of the transmission coefficient and localization length for an exact palindromic sequence are shown in Fig. 3.10. The main difference between the palindromic and periodic or mismatched sequences is that the formation of many minibands with many gaps in the transmission appears. As the temperature increases, the magnitude of the transmission is reduced and the width of gap becomes larger. As mentioned earlier, the temperature effects lead to destruction of phase coherence in the transmission and reduce the mean transmission coefficient due to the quantum interference. We conclude that the thermal fluctuations affect drastic changes in transmission coefficient as well as localization length in the exact palindromic DNA sequence.
Fig. 3.10. Transmission coefficient and localization length as a function of electron energy for a palindromic DNA sequence at various temperatures.

3. 6. **I-V characteristics for different sequences of DNA**

The nature of DNA sequences can influence the electron transmission. We now examine the current-voltage characteristics for periodic, mismatched, and palindromic sequences. We
evaluate $I-V$ characteristics of the three sequences with transmission coefficient $T(E)$, using Eq. (2.8) at room temperature. The $I-V$ characteristics vary with the relative values of the Fermi energy because the Fermi energy window mainly contributes to the conduction. Here, we choose $E_f = 5.75\,\text{eV}$ and $\eta = 0.5$. The $I-V$ curves in Fig. 3.11 show a negligible current until it reaches a threshold voltage. Once it reaches to a threshold voltage, the current displays a sharp rise that is a feature of semiconductor. It is clear that when $V_{sd} > 3$ volts, periodic sequence (blue curve) of poly(G)-poly(C) ds-DNA shows a higher current than the mismatched and palindromic sequences.

Fig. 3.11. $I-V$ characteristics with $E_f = 5.75\,\text{eV}$ with different sequences of DNA.
Chapter 4: Spin polarization properties through double-stranded DNA

4.1. Introduction

The spintronics field focuses on the employment of electron spin for data storage and processing purposes. Most current spintronic devices are based on inorganic materials, but the use of organic materials in spintronics has become a popular topic in scientific society [77, 78]. In the last two decades, scientists have studied the fundamental properties of electrons in order to develop materials that produce greater computational speeds but consume less power. Electron spin, a quantum property of electrons, is one of these properties; it is referred to as spin-up if it rotates counter-clockwise, spin-down if clockwise.

In recent years, researchers have made many studies in hopes of developing spintronic devices out of chiral molecules such as double-stranded DNA. Experimentally, Gohler et al. recorded the spin-selective transmission of the electron through monolayers of dsDNA at room temperature, as shown in Fig. 4.1 [79]. They observed an efficient spin filtration and noted that spin polarization increases with dsDNA length. Later, Xie et al. measured charge transport through double-stranded DNA oligomers connected to two electrodes [80]. They discovered that dsDNA molecules could act as very efficient spin filters. Similarly, Mishra et al. found spin-dependent effects in single-helical bacteriorhodopsin connected to gold and aluminum substrates [81].
These experimental studies have prompted intense interest in the use of organic materials in spintronic applications. A theoretical study, employing the Bogoliubov–de Gennes (BdG) equations and the non-equilibrium Green’s function (NEGF) method, focused on evaluating spin polarization and spin-dependent electron conductance on the dsDNA’s helical symmetry, length, and environment-induced dephasing factors. The results showed that the conductance is inversely proportional to the DNA’s length and environment-induced dephasing factors, with spin polarization depending on the DNA’s length and helical symmetry [82]. A high spin polarization also became evident in the well-organized monolayers of lengthy DNA molecules by studying spin-orbit coupling, environment-induced dephasing, and helical symmetry. Self-assembled monolayers of DNA molecules along a gold electrode produced a notable spin polarization that extends up to 60%, provided that it remained under room temperature [83]. A similar result was
observed when the double-stranded DNA molecules were squeezed together between electrodes [82, 83]. In addition, a study involving the spin polarization calculation using the Landauer-Büttiker formula expounded that spin polarization is also dependent on the DNA’s magnitude, DNA’s length, and the gate voltage. In the case of a long DNA molecule, the spin polarization could reach beyond 70% as long as the gate voltage remained properly tuned [84]. Approximately the same percentage was found when Li et al. studied the magnetoresistance ($R_m$) of a double-stranded DNA molecule. Magnetoresistance magnitude attained up to 72.5% for DNA when a spin-orbit coupling with helix spring geometry was considered [78]. Additionally, DNA molecules, specifically those with numerous base-pairs, are also heavily involved in inducing spin polarization when the spin-orbit coupling and helical symmetry are taken into account [83, 85]. Even in the presence of a multi-terminal structure, where one terminal works as a source while the others act as a drain, spin polarization is observed. In this study, the behavior of parallel strength but opposite directions was recognized, thereby allowing spin polarization and spin separation to be realized simultaneously [86]. These studies demonstrate that DNA, in both natural and artificial sense, serves as a perfect spin filter over a wide range of parameters. Although spin polarization can occur in double-stranded DNA, a single-stranded DNA shows an absence of spin polarization [84, 85, 86]. In this case, certain restrictions that could either be linked to non-magnetic leads or impaired by ultraviolet light [79, 83] must be applied to observer spin polarization.

Motivated by these results, we consider a two-dimensional (2-D) DNA linked between two semi-infinite electrodes which provides four possible channels. We calculate the spin-dependent transmission and spin polarization of finite lengths of dsDNA, using a tight-binding (TB) model. We discuss in detail the general factors that affect spin-dependent transmission and spin polarization, such as spin-orbit coupling $t_{so}$, DNA lengths, helix angle $\theta$, and twist angle $\varphi$. We
show overall 2-D and 3-D contour plots of the transmission up (or down) and spin polarization with variations of spin-orbit coupling, DNA lengths, helix angle, and twist angle. We compare the spin polarization of the homogeneous sequence to that of the mismatched sequences. Finally, we calculate the spin-polarized current (or net spin current) for different values of spin-orbit coupling and helix angle using the Landauer-Büttiker formula.

4. 2. Model

We consider a double-helix structure of DNA molecules attached to semi-infinite leads (electrodes) in the presence of an electron spin effect. Our DNA structure consists of finite number of nucleotides which are connected by hopping amplitude; \((t_{i,i+1},T_{i,i+1})\) between the bases, \((V_{L1,L2}, V_{R1,R2})\) to the leads, \((h_i)\) between the base-pairs, \((V_a)\) to the upper (lower) backbone sites, and \((B_a)\) intra-backbone (see Fig. 4.2). The circles in the DNA structure illustrate the base-pairs, while the hexagons represent the backbone (phosphate and sugar groups). Each base has an energy given by the ionization potentials; \(G = 7.75 \text{ eV}, C = 8.87 \text{ eV}, A = 8.24 \text{ eV}, T = 9.14 \text{ eV}\) and the backbone has an energy of \(8.5 \text{ eV}\). The arrows represent the two possible ways of electron spin transmission through dsDNA. Red arrows define spin-up, while green arrows for spin-down.
The effective Hamiltonian for electron spin transport through the dsDNA between two metallic leads can be written as

$$H_{Tot} = H_{DNA} + H_{Leads} + H_{Leads-DNA} + H_{SO}. \quad (4.1)$$

The total Hamiltonian is divided into four parts: the DNA itself, the leads themselves, the coupling between the DNA and the leads, and the spin-orbit part. The Hamiltonian of the DNA, including the spin degree of freedom, is expressed as

$$H_{DNA} = \sum_{n,j} (e_n c_{n,j}^\dagger c_{n,j} + e_j d_{n,j}^\dagger d_{n,j} + e_a a_{n,j}^\dagger a_{n,j} + e_a b_{n,j}^\dagger b_{n,j}) - \sum_n (V_a c_{n,j}^\dagger a_{n,j} + V_a d_{n,j}^\dagger b_{n,j} + h_n c_{n,j}^\dagger d_{n,j} + h.c.) - \sum_{n,\sigma} (t_{(n,n+1)\sigma} d_{n,\sigma}^\dagger d_{n+1,\sigma} + T_{(n,n+1)\sigma} c_{n,\sigma}^\dagger c_{n+1,\sigma} + B_{a,\sigma} a_{n+1,\sigma}^\dagger a_{n,\sigma} + B_{a,\sigma} b_{n,\sigma}^\dagger b_{n+1,\sigma} + h.c.), \quad (4.2)$$

where \((c_{n,j}^\dagger c_{n,j})_\sigma, (d_{n,j}^\dagger d_{n,j})_\sigma, (a_{n,j}^\dagger a_{n,j})_\sigma\) and \((b_{n,j}^\dagger b_{n,j})_\sigma\) are the creation (annihilation) operators of the spinor \(\sigma = (\uparrow, \downarrow)\) on the \(n\)-th site of a DNA molecule whose length is \(N\) bases, \(j\).
labels the helical chain, \(e_n, e_j\) are the on-site potential energies of the DNA bases, and \(e_a\) is the on-site potential energy of the backbone. The Hamiltonian of the electrodes themselves can be described as

\[
H_{Leads} = \varepsilon_0 \sum_{n \leq 0 \text{ and } n > N} t_n^\dagger t_n - V_0 \sum_{n \leq 0 \text{ and } n > N} (t_n^\dagger t_{n+1} + \text{h.c.}),
\]

where the lead on-site energy is \(\varepsilon_0 = 7.75\) eV and intrachain lead is taken as \(V_0 = 1\) eV. The DNA molecule is coupled to two semi-infinite electrodes by the tunneling Hamiltonian:

\[
H_{Leads-DNA} = -V_{L1} l_{0,\sigma}^\dagger c_{1,\sigma} - V_{L2} l_{0,\sigma}^\dagger d_{1,\sigma} - V_{R1} l_{1,\sigma}^\dagger c_{N,\sigma} - V_{R2} l_{1,\sigma}^\dagger d_{N,\sigma} + \text{h.c.},
\]

where \(V_{L1}\) and \(V_{L2}\) are the coupling strength connecting the DNA molecule with the left electrode, while \(V_{R1}\) and \(V_{R2}\) are that connecting the DNA molecule with the right electrode.

The spin-orbit (SO) Hamiltonian is described by [78, 83].

\[
H_{so} = \sum_{\sigma = \uparrow, \downarrow} \sum_{n = 1}^{N} t_{so} \sum_{j = 1}^{4} l_{j,n}^\dagger l_{j,n+1} [\sigma_n^j + \sigma_{n+1}^j] + \text{h.c.},
\]

where, \(t_{so}\) is the spin-orbit coupling (SOC) strength, and the terms inside the square bracket can be expressed by the following equation:

\[
\sigma_n^j = \sigma_x \sin[(n-1)\phi + (j-1)\pi] \sin \theta - \sigma_y \cos[(n-1)\phi + (j-1)\pi] \sin \theta + \sigma_z \cos \theta,
\]

where \(\sigma_x, \sigma_y, \text{ and } \sigma_z\) are Pauli matrices, \(\phi\) is the twist angle, and \(\theta\) is the helix angle. After solving Eq. (4.5), we arrive at a 2 x 2 matrix,

\[
\begin{bmatrix}
A_{j,n} & B_{j,n} \\
C_{j,n} & D_{j,n}
\end{bmatrix}.
\]

The elements of the matrix can be written as follows:
\[ A_{j,n} = 2\, t_{so} \cos \theta_{jn}. \]
\[ D_{j,n} = -2\, t_{so} \cos \theta_{jn}. \]
\[ B_{j,n} = t_{so} \sin \theta [\sin ((n - 1) \varphi + (j - 1) \pi) + \sin [n \varphi + (j - 1) \pi] + i \cos [(n - 1) \varphi + (j - 1) \pi] + i \cos [n \varphi + (j - 1) \pi]]. \]
\[ C_{j,n} = t_{so} \sin \theta [\sin ((n - 1) \varphi + (j - 1) \pi) + \sin [n \varphi + (j - 1) \pi] - i \cos [(n - 1) \varphi + (j - 1) \pi] - i \cos [n \varphi + (j - 1) \pi]]. \]

We apply the wave functions into the tight-binding (TB) Schrödinger equations for our dsDNA structure, and then arrange the solutions in a matrix form. The matrix that includes the electron spin becomes twice as large as the matrix without spin. By solving the matrix for total Hamiltonian, we get the transmission amplitude as a function of incoming electron energy, \( t_{\uparrow(\downarrow)}(E) \). The transmission coefficient for spin (\( \uparrow \) or \( \downarrow \)), is obtained by taking the absolute square of transmission amplitude \( t_{\uparrow(\downarrow)}(E) \).

\[ T_{\uparrow} = |t_{\uparrow}(E)|^2 \text{ and } T_{\downarrow} = |t_{\downarrow}(E)|^2. \] (4.7)

4.3 Spin polarization of dsDNA

The spin polarization, which is ratio of the electron transmission up (\( \uparrow \)) and down (\( \downarrow \)), is used to extract the degree of spin-state transmission. To understand the role of asymmetry on spin-selective transport through the DNA molecule, we calculate spin polarization using the following equation:
\[ P_s = \frac{T_\uparrow - T_\downarrow}{T_\uparrow + T_\downarrow}, \]  
\[ (4.8) \]

where \( T_\uparrow \) is the transmission probability for a spin-up and \( T_\downarrow \) is the transmission probability for a spin-down. \( P_s = 0 \) means there is no spin polarization, but \( P_s = -1 \) (+1) means that the degree of down (up) spin polarization is 100\% [87].

**4.3.1. The dependence of spin-orbit coupling (SOC) on spin polarization**

In this section, we calculate the spin-dependent transmission and spin polarization of five base-pairs of poly(G)-poly(C) DNA sequence in the absence and presence backbone effects. Because the spin-orbit coupling SOC \( (t_{so}) \) connects the electron spin to the charge degree of freedom [87], we investigate the effect of it on both spin-related transmission \( (T_\uparrow \) and \( T_\downarrow \)) and spin polarization \( P_s \). For numerical calculation, we choose the parameters of the system as follows: 
\[ t_{i,i+1} = T_{i,i+1} = 0.1 \text{ eV}, \quad h_i = 0.2 \text{ eV}, \quad \text{and} \quad V_{L1,L2} = V_{R1,R2} = 0.2 \text{ eV}. \]
Moreover, the other two parameters related to the spin part are chosen as \( \theta = 37.8^\circ \) and \( \varphi = 36^\circ \) because these parameterizations are demonstrated to obtain large spin polarization [86]. We choose some typical values of the SOC strength \( (t_{so}) \) to investigate the spin-selective transmission and spin polarization coefficient in two different cases.

First, we display the transmission probability of the spin-up (down) electron and spin polarization in the absence of backbone effects. The spin-dependent transmission \( T_\uparrow \) and \( T_\downarrow \) are presented in Fig. 4.3 for four different SOC strengths \( (t_{so} = 0.01, 0.05, 0.1, \text{ and } 0.4 \text{ eV}) \). At a small value of \( t_{so} \), two mini-bands appear in the transmission spectrum separated by a band gap in both \( T_\uparrow \) and \( T_\downarrow \). When SOC \( (t_{so}) \) values increase, two well-separated mini-bands are mixed together, and distinct resonant peaks appear in the spin-dependent transmission of \( T_\uparrow \) and \( T_\downarrow \). Especially it is interesting to note that for \( t_{so} = 0.05 \text{ eV} \), spin-up transmission vanishes.
completely, and spin-down transmission shows well-arranged two mini-bands with under-unity resonant peaks. The contour plots [see Fig. 4.3 (b) and (d)] clarify that increasing $t_{so}$ value makes a collapse of mini-bands, and reform well-separated and distinct resonant peaks in the spin-dependent transmission of $T_\uparrow$ and $T_\downarrow$.

Fig. 4.3. Spin-dependent transmissions and contour plots for (a, b) spin-up and (c, d) spin-down at different $t_{so}$ values without backbone effects.

When the spin-up transmission $T_\uparrow$ differs from the spin-down transmission $T_\downarrow$, the spin polarization $P_S$ is nonzero. Figure 4.4(a) plots the spin polarization $P_S$ as a function of incoming energy $E$ with different SOC ($t_{so}$) values in the absence of backbone effects. At $t_{so} = 0.01$ and 0.1 eV, the spin polarization bands can be found around the area of the on-site energy of the DNA's bases ($E = 7.75$ and 8.87 eV). It is clearly seen that increased $t_{so}$ leads to achievement of 100%
spin polarization $P_s$, where the spin polarization oscillates from a perfect spin-up and spin-down. To show a clearer picture, we plot two-and three-dimensional graphs of the spin polarization as a function of electron energy $E$ and spin-orbit coupling $t_{so}$ (see Fig. 4.4(b and c)). We conclude that high SOC ($t_{so}$) strength leads to large spin polarization.

![Figure 4.4](image)

Fig. 4.4. (a) Spin polarization vs electron energy, (b) contour plot of spin polarization vs electron energy, and (c) 3-D contour plot of spin polarization vs electron energy for different values of $t_{so}$ in the absence of backbone effects.

The sugar-phosphate backbone plays an important role in the nucleic acid structure; it has consecutive single bonds with substantial independence for correlated torsional rotations [88].
Considering and studying the backbone effect, both experimentally and theoretically, has become a focus of recent research [88, 89]. Motivated by this idea, we evaluate the spin-dependent electron transmission and spin polarization along five poly(G)-poly(C) DNA for different values of $t_{so}$ by taking the backbone effect into consideration. We consider the hopping integral between DNA and upper (lower) backbone $V_a = 0.1$ eV as well as the hopping along backbone sites $B_a = 0.1$ eV shown in Fig. 4.2. Spin-up transmission $T_\uparrow$ $vs$ $E$ and spin-down transmission $T_\downarrow$ $vs$ $E$ are displayed in Fig. 4.5(a) and (c) for $t_{so} = 0.01, 0.05, 0.1, \text{ and } 0.4$ eV. Both $T_\uparrow$ and $T_\downarrow$ show extra peaks of mini-band at $E = 8.5$ eV which is the backbone on-site energy. As $t_{so}$ increases, these extra peaks spread out widely over a range of energy and merge with the rest of the peaks in the transmission. The contour plot also indicates that increasing $t_{so}$ leads to an overlapping of transmission bands (both $T_\uparrow$ and $T_\downarrow$) and a collapse of minibands, which generates distinct resonant peaks over a wide range of energy. The dotted white line in the contour plot of $T_\uparrow$ indicates a merging of resonant peaks approximately at $t_{so} = 0.054$ eV, after which the $T_\uparrow$ spreads out broadly in an energy range.
Because effective spin polarization requires high transmission, we choose to open the backbone couplings to increase the transmission probability. The spin polarization $P_S$ is plotted at different values of $t_{so}$ as shown in Fig. 4.6. At $t_{so} = 0.01$ eV and 0.1 eV, spin polarization oscillates between $-1$ to $+1$ around $E = 8.5$ eV, showing that the degree of up or down $P_S$ is $\sim 100\%$. At $t_{so} = 0.4$ eV, however, the positions of perfect spin polarization $P_S$ change and spread out a wide range of energy. It is evident that the efficiency of spin filtration is quite large for all investigated values of $t_{so}$ with backbone effect. Our analysis of Fig. 4.4 and Fig. 4.6 verify that dsDNA, even when $t_{so}$ is weak, can act as a perfect spin filter; this finding agrees well with the experimental [79, 80] and theoretical works [82, 83].
Fig. 4.6. (a) Spin polarization $P_S$ as a function of the incoming electron energy $E$, (b, c) 2-D and 3-D contour plot of spin polarization $P_S$ as a function of $E$ and $t_{so}$ with backbone effects.

4.3.2. Variation of spin-orbit coupling, helix angle, and twist angle

The overall goal in our work is to characterize the spin polarization of a long chain of dsDNA. We increase the number of poly(G)-poly(C) base-pairs from five to twenty in the presence of backbone effects. The spin polarization $P_S$ can be calculated as a function of the incoming electron energy, using Eq. (4.8) at fixed parameters: $t_{i,i+1} = T_{i,i+1} = 0.2$, $h_i = 0.2$, $V_{L1,L2} = V_{R1,R2} = 0.3$, $V_a = 0.1$, and $B_a = 0.1$ in unit of eV. In general, when we consider a longer
dsDNA, more peaks in the transmission arise and then more rich behaviors spin polarization are expected. Our study shows that an increase in dsDNA length leads to significant enhancement of spin filtration efficiency; this agrees with other studies [79, 83, 85]. Because the SOC $t_{so}$, helix angle $\theta$, and twist angle $\phi$ are sensitive to the charge distribution in DNA and the properties of the surrounding environment, we make a detailed study and comprehensive analysis of the effects of all these factors on spin-selective transmission. If any of these factors are absent, then no spin polarization is visible. First, we examine the spin polarization $P_S$ along 20 poly(G)-poly(C) base-pairs of dsDNA at selected values of $t_{so}$, as shown in Fig. 4.7(a) and (b). At $t_{so} = 0.01$ and 0.05 eV, the spin polarization is reasonably large in most energy regions comparing to the same situation of five base-pairs. We notice that perfect spin polarizations are distributed to a wide range of energy at $t_{so} = 0.05$ eV.

We also discuss the dependence of spin polarization on twist angle $\phi$ and helix angle $\theta$, as shown in Fig. 4.7(c, d, e, and f). The helix and twist angles of dsDNA can vary like those of a spring in a proper environment or under external stress and torque. Figure 4.7(c and d) show the results for two values of twist angle ($\phi = 30^\circ$ and $45^\circ$, respectively), maintaining a fixed $t_{so} = 0.01$ eV and $\theta = 37.8^\circ$. At $\phi = 30^\circ$, the $P_S$ shows sharp polarization spikes around $E = 8.5$ eV and a collection of bipolar spin polarization is concentrated on this energy area. In the meantime, the transmission at $E \approx 7.4$ eV is polarized spin down unlike the case of Fig. 4.7(a). When $\phi = 45^\circ$ the spin-up polarization at $E \approx 7.4$ eV is enhanced by approximately 50%. Finally, we plot the spin polarization $P_S$ for different helix angle $\theta$ with fixed $t_{so}$ and $\phi$, as shown in Fig. 4.7(e and f). We note that $P_S$ at $\theta = 75^\circ$ shows less sharp polarization spikes at $E \approx 7.4$ eV and $E \approx 9.3$ eV and is slightly smaller than that at $\theta = 30^\circ$. Interestingly, the plots in Fig. 4.7 show that variation
of any of the three factors (SOC $t_{so}$, helix angle $\theta$, and twist angle $\varphi$) could lead to significant changes in spin polarization $P_S$.

Fig. 4.7. Spin polarization versus electron energy for different (a, b) SOC ($t_{so}$), (c, d) twist angle $\varphi$, and (e, f) helical angle $\theta$. 
4. 3.3. Mismatched sequences

Electron transport through DNA is mainly affected by the on-site energy of the nucleotide and hopping integrals between bases. Here, we focus on studying the change in on-site energy caused by a defect in the DNA sequence—the replacement of one nucleotide by another. This defective or mismatched sequence is represented by a variation in the conformation of base-pair G-T, C-A, C-T, or G-A. The mismatched sequence, which causes a change in DNA structure, also influences electron transmission through the DNA molecule [90]. The electron transmission through different mismatched sequences of DNA has been investigated both experimentally [91] and theoretically [92]. It was shown that the replacement of base-pairs by mispairs in DNA sequence can suppress the charge transmission [91]. Guo et al. found that the spin sensitivity of spin-dependent transmission through dsDNA strongly depends on the DNA sequence and is controlled by its end segment [85]. Motivated by this study [85], we evaluate the effect on spin polarization $P_S$ of increasing the number of poly(G)-poly(T) mispairs in the middle of a homogeneous poly(G)-poly(C) DNA sequence.

Figure 4.8 represents the energy dependence of the spin polarization $P_S$ in the DNA: (a) a homogeneous poly(G)-poly(C) sequence, (b) two poly(G)-poly(T) mispairs, (c) four poly(G)-poly(T) mispairs, and (d) eight poly(G)-poly(T) mispairs in the middle of the DNA sequence. Here, the parameters are set as follows: $t_{i,i+1} = T_{i,i+1} = 0.2$ eV, $h_i = 0.2$ eV, $V_{L1,L2} = V_{R1,R2} = 0.3$ eV, $V_a = 0.1$ eV, $B_a = 0.1$ eV, $t_{so} = 0.01$ eV, $\theta = 37.8^\circ$, and $\varphi = 36^\circ$. The spin polarization of each mismatched sequence differs slightly from that of the homogeneous poly(G)-poly(C) sequence; the difference is due to the change of on-site energies. Because the on-site energy of cytosine (C) is replaced by the on-site energy of thymine (T), the modification of the on-site energy includes only the cytosine (C) base, not the guanine (G) base. This replacement causes the appearance of
additional oscillations in spin polarization, especially in the energy range $E \geq 9$ eV, as shown in Fig. 4.8(b, c, and d). As Fig. 4.8 makes clear, the spin polarization remains the same in the energy regions of the guanine (G) and backbone strands and changes only in the energy region of the cytosine (C) strand. Inserting two mispairs into the DNA sequence, as shown in Fig. 4.8(b), does not make a big alteration in spin polarization. However, increasing the number of poly(G)-poly(T) mispairs from two to eight base-pairs can enhance the spin polarization to almost 50% at $E \approx 9.14$ eV. In this situation, no strong reduction due to the position of poly(G)-poly(T) mispairs is evident in the energy dependence of the spin polarization. It can be concluded that spin polarization has a weak dependence on the position of mispairs when the replacement occurs at a distance from the contacts (leads); this agrees with Apalkov et al.’s results [93].

Fig. 4.8. Energy-dependent spin polarization $P_S$ for 20 base-pairs (a) in a homogeneous poly(G)-poly(C), (b) with two poly(G)-poly(T) mispairs, (c) with four poly(G)-poly(T) mispairs, and (d) with eight poly(G)-poly(T) mispairs in dsDNA sequence.
4.4. Net spin current

The measurement of spin-polarized current (or pure spin current) is one of the many interesting challenges in the study of spin-dependent transmission. Pure spin current, \( P_{\text{current}} \), is the flow of electron spin angular momentum without a simultaneous flow of electric charge. Composed of electron spin-up current and spin-down current, \( P_{\text{current}} \) can play an important role carrying and storing information in spintronic devices. Realization of efficient spin injection in such devices has generated widespread interest in scientific fields [94]. For example, quantum dot-based devices have been studied to investigate transmission of spin-polarized current [95, 96]. Similarly, Rai and Galperin have suggested a way of generating pure spin current in the DNA that can help to measure spin currents in organic nano-devices [97].

Here, we shed light on basic aspects of investigating pure spin current \( P_{\text{current}} \) through poly(G)-poly(C) dsDNA. In order to calculate \( P_{\text{current}} \), we first obtain the electrical current for spin-up and spin-down electrons directly by using the Landauer-Büttiker formula at room temperature:

\[
I_{T(l)} = \frac{2e}{h} \int_{-\infty}^{\infty} T_{T(l)}(E) \left[ f_L(E) - f_R(E) \right] dE, \tag{4.9}
\]

where \( T_{T(l)}(E) \) stands for the spin-dependent transmission function calculated by using Eq. (4.7), \( e \) is the electronic charge, \( h \) is the Planck constant, and \( f_L(f_R)(E) = 1 / \{ e^{[(E-\mu_{L(R)})/k_B T]} + 1 \} \) is the Fermi distribution function. The chemical potential of the left (right) electrode is denoted by \( \mu_{L(R)} \) and depends on the applied bias. According to Datta et al., we set the chemical potential to \( \mu_L = E_f + (1 - \eta) eV_{sd} \) and \( \mu_R = E_f - \eta eV_{sd} \), where \( E_f \) is the equilibrium Fermi energy, \( V_{sd} \) is applied bias voltage, and \( \eta \) describes an asymmetry parameter of contact to leads [98]. In our
calculations, we choose the parameters as follows: $E_f = 8.3$ eV and $\eta = 0.5$. Using Eq. (4.9), the spin current $I_S$ and charge current $I_C$ are defined as following equations:

$$I_S = I_\uparrow - I_\downarrow.$$

$$I_C = I_\uparrow + I_\downarrow.$$

We use the above two equations to calculate the spin polarization of the current, $P_{\text{current}}$, as

$$P_{\text{current}} = \frac{I_S}{I_C}. \quad (4.10)$$

In order to understand spin-dependent conductance, we study the pure spin current or fully spin-polarized current $P_{\text{current}}$ in 20 base-pairs of dsDNA in the presence of backbone effect. The spin-exchange interactions between electrons and DNA allow us to study the current-voltage (I-V) characteristics and corresponding spin-polarized current $P_{\text{current}}$ under the influence of spin-orbit coupling $t_{so}$ and helix angle $\theta$. First, we calculate I-V characteristics and the differential conductance ($dI/dV$) as a function of source-drain applied voltage $V_{sd}$ for three different values of $t_{so} = 0.01, 0.1,$ and $0.4$ eV in Fig. 4.9(a, c, e). In addition, we examine the effect of the variation of the SOC $t_{so}$ on spin-polarized current $P_{\text{current}}$ as a function of bias voltage $V_{sd}$ with fixed helix angle $\theta = 37.8^\circ$ and twist angle $\varphi = 36^\circ$ in Fig. 4.9(b, d, f). For $t_{so} = 0.01$ eV, as illustrated in Fig. 4.9(a), the spin-up current is slightly higher than the spin-down current when $V_{sd} > 1.8$ V. For both spin-up and spin-down currents, the I-V curves show a negligible current until it reaches to a threshold voltage of $V_{sd} \approx 1.8$ V and then it remains constant. This certainly is a typical characteristic of semiconductor with a current gap of $3.6$ V. The differential conductance shows a double-peak structure with an amplitude of $\sim 55 \mu A/V$ for spin-up current and $\sim 45 \mu A/V$ for spin-
down current [see the insets of Fig. 4.9(a)]. We find in Fig. 4.9(b) that, under a small bias voltage, the spin polarization current increases rapidly until it reaches close to 80%.

Fig. 4.9. Spin-up current $I_\uparrow$ and spin-down current $I_\downarrow$ with corresponding differential conductance curves (a, c, and e) and spin polarization current $P_{\text{current}}$ (b, d, and f) versus bias voltage $V_{sd}$ for selected values of SOC $t_{so} = 0.01, 0.1,$ and $0.4$ eV.
We also plot the $I-V$ characteristics as a function of voltage for spin-up $I_\uparrow$, spin-down $I_\downarrow$, and spin polarization current $P_{\text{current}}$ in the case of $t_{so} = 0.1$ eV [see Fig. 4.9(c and d)]. We can see that spin-down $I_\downarrow$ is dramatically increased in comparison with spin-up $I_\uparrow$. Therefore, the value of the spin-dependent current forms in a negative field and plunges to $-1$ near zero applied voltage, while still achieving highly efficient spin-down filtering of $\sim100\%$. We observe that spin-down $dI/dV$ displays a double peak structure with a reduced amplitude and a broaden peak width in comparison with spin-up differential conductance [see the insets in Fig. 4.9(c)]. With an increase in SOC to $t_{so} = 0.4$ eV, the spin-up current increases rapidly and the spin-down current is partially suppressed with a step-like current jumps, as shown in Fig. 4.9(e). Both spin-up and spin-down currents exhibits an Ohmic behavior with no current gap that is a typical signature of metal. In both spin-up and spin-down $dI/dV$ plots, conductance oscillations as a function of $V_{sd}$ appear in the inset in Fig. 4.9(e). Each peak of the conductance oscillations correspond to each current step present in the corresponding $I-V$ curve. The magnitude of these peaks in spin-down $dI/dV$ is suppressed approximately three times than that of spin-up one. Spin polarization of current $P_{\text{current}}$ ranges a polarization between 40% and 70% except around $V_{sd} = 0$, where it is almost 0% as shown in Fig. 4.9(f). It is interesting to note that when we increase the SOC ($t_{so}$), spin current and corresponding differential conductance and spin filtration efficiency change significantly.

Finally, we study the effect of modulating the helix angle $\theta$ on spin-polarized current $P_{\text{current}}$ of dsDNA. Charge current $I_C$, spin current $I_S$, and spin-polarized current $P_{\text{current}}$ versus applied voltage $V_{sd}$ are presented in Fig. 4.10 for selected helix angles ($\theta = \pi/4$ and $\pi/6$) at a
fixed \( t_{so} = 0.01 \text{eV} \). The observation of \( I_C \) curves for \( \theta = \pi/4 \) and \( \pi/6 \) shows that dsDNA molecules have typical characteristics of a semiconductor with a large differential conductance \( dI_C/dV \), as shown in Fig. 4.10(a and d) [see also insets]. In the meantime, \( I_S \) shows an abrupt change in current (Fano shape) at \( V_{sd} = \pm 1.5 \text{V} \) in Fig. 4.10(b and e), while \( I_C \) increases smoothly at the same voltage. The differential conductance \( dI_S/dV \) as a function of an applied voltage is depicted in insets in Fig. 4.10(b and e), where the magnitude of conductance oscillations is approximately 20 \( \mu \text{A/V} \). Combining \( I_C \) and \( I_S \) from Eq. (4.10), we show in Fig. 4.10(c) that the current is fully polarized spin-down and spin-polarization current \( P_{current} \) for \( \theta = \pi/4 \) reaches to \( \sim 80\% \) at \( V_{sd} = \pm 0.6 \text{V} \), while \( P_{current} \) is zero at \( |V_{sd}| > \pm 1.5 \text{V} \). When \( \theta = \pi/6 \), bipolar spin polarization is demonstrated with a small value of \( V_{sd} = \pm 0.8 \text{V} \) in Fig. 4.10(f). Here, the spin-dependent current produces a polarization of \( P_{current} = 80\% \) for spin up and \( P_{current} = 40\% \) for spin-down.
Fig. 4.10. The charge current $I_C$, spin current $I_S$, and spin-polarized current $P_{\text{current}}$ as a function of source-drain $V_{sd}$ for different helix angles $\theta$. The insets show the differential conductance $dI/dV$ for $I_C$ and $I_S$ at $\theta = \pi/4$ and $\pi/6$. 
Chapter 5: Summary and Conclusion

In this work, we numerically evaluated the electron transmission properties through DNA molecules using the two-dimensional (2-D) four-channel model. We investigated the effect of the magnetic field, temperature, and electron spin on the electron transport through a finite length of DNA molecules using tight-binding (TB) Schrödinger equation.

In Chapter 2, we examined the electron transmission by applying the magnetic field in the hopping integrals of DNA structure. We also studied the different length of the poly(G)-poly(C) DNA molecules when exposed to the variations on backbone effects, hydrogen bonds, and contact leads. The results showed that the number of loops in the DNA structure increased as the hydrogen bonds and the number of base-pair expanded. This also suggested that a direct proportional relationship exists between the periodicity and the number of loops. Furthermore, the presence of backbone effects doubled the periodicity of the AB oscillations and increased the electron transmission, while the periodicity of AB oscillations remained unaffected by the changes in the coupling between leads and DNA. We showed the periodicity of AB oscillations in electron transmission through DNA by changing the value of the applied magnetic field. A semiconductor behavior has been observed in the presence of an external magnetic field.

In Chapter 3, we focused our attention to the impacts of temperature on the electron transmission properties through double-stranded DNA. Periodic, mismatched, and exact palindromic sequences have been employed to determine the electron transmission and $I$-$V$ characteristics under the effect of thermal fluctuations. For the periodic sequence, the increase in temperature created disorder in the system and reduced the localization length; thus, diminishing the electron conductance. Like the periodic sequence, the electron transmission and localization
length in the mismatched sequence are affected by thermal fluctuations. In the mismatched sequence, we also examined the temperature effect for different Fermi energy. For the exact palindromic sequence, the thermal fluctuations also lead to the destruction of phase coherence in the transmission coefficient and make the localization lengths smaller. We showed that the periodic sequence demonstrated the highest current among the mentioned sequences.

Finally, in Chapter 4, we investigated the spin-dependent transmission and spin polarization of a finite length of dsDNA. The investigation also included the general factors that affected the spin-dependent transmission and spin polarization such as the spin-orbit coupling, DNA lengths, helix angle, and twist angle. In terms of spin polarization, the findings of this thesis confirmed that the double-stranded DNA serves as a perfect spin filter even for the weak spin-orbit coupling. The spin filtration efficiency of dsDNA could be greatly enhanced by the increase of DNA length. It should be noticed that the existence of the spin-orbit coupling, helix angle, and twist angle would be necessary to generate spin polarization in DNA. We also observed that the mismatched sequences have little effect on the spin polarization when the mispairs replaced away from the DNA-lead coupling. Such little effect could be attributed to the changes in on-site energies (i.e. from C to T). The on-site energy in our system remained the same for all regions except for the C strand because we replaced poly(C) by poly(T). However, increasing the number of poly(G)-poly(T) mispairs in the middle of the sequence can enhance the spin polarization.

As for the spin-dependent transmission, the varying spin-orbit coupling could influence the spin-polarized current. We found that the spin-polarized current could rapidly increase under a small bias voltage and the double-stranded DNA can act as a semiconductor behavior at the small spin-orbit coupling. However, given the high value of spin-orbit coupling, the spin-up and spin-down currents show an Ohmic behavior with high spin-polarized current. It should be noticed that
the increase in spin-orbit coupling could significantly alter the DNA conductance and filtration efficiency. The modulation of the helix angle also affected the spin-polarized current such that the charge current showed a semiconductor behavior with a high percentage of spin-polarized current ~80%.

Our study opens the possibility of using the dsDNA as a component in the spintronics devices. For future analysis, we need to examine the spin polarization on poly(T)-poly(A) sequence. More than that, the study on spin polarization should also expand through the mismatched sequences when the replacement of mispairs appear near to the contacts (DNA-lead coupling). We will also consider the effect of the external magnetic field and thermal fluctuations on the spin polarization and spin-polarized current in DNA molecules.
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