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Spintronics in nano scales: An approach from DNA spin polarization

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Abstract. DNA nanotechnology is a purist approach to biomolecular engineering. The field is aimed to create molecular structures and devices through the exclusive use of DNA as an engineering material. On the other hand, DNA Spintronics, as a DNA nanotechnology field, uses the electron spin to store and process information. In this work, we have used the Peyrard-Bishop-Holstein model combined with spin-orbit interaction for studying the spin transfer mechanism in DNA nanowires. In this work, the electrical currents corresponding to the spin-up and spin-down electrons are obtained directly using the Hamiltonian equations of system. We can obtain the best functional ranges for external agents, such as magnetic and electrical fields, and surroundings temperature to use in spintronics applications. By considering the simultaneous effects of parameters, we have determined the islands with pure spin current. However, the considerable result is where we have applied the time periodic magnetic field and observed the characteristic peaks in polarization diagram. These peaks can be used for information coding as zero-one codes. Therefore, one could construct DNA nanowires that filter the spin current, create the nearly pure spin currents, and act as a spintronics device for processing and transferring information.

1. Introduction

DNA as a molecule that carries the genetic information of a living organism is diverse in structure and function. In nature, this complementary base pairing contributes to DNA's helical structure and the way genetic information is stored and retrieved. Because of its programmability, DNA has also earned itself a reputation as a versatile engineering material. The well-characterized nature of DNA base pairing provides an easy means to control DNA interactions; this 'sequence programmability' has allowed the rational design of precisely defined structures, and molecular motors or circuits that can autonomously move or process information. In the last 30 years, the DNA nanotechnology community has gone from an initial wave of making static structures of different shapes and sizes to a second wave of creating increasingly sophisticated and dynamic structures capable of carrying drugs, interacting with cell surface proteins, and performing certain functions inside cells [1,2]. In the case of dynamic structures, such as those that can move or perform computational tasks, strand displacement is used, whereby the nanodevice is programed to respond to an incoming DNA strand that displaces an existing one on the nanodevice [3]. The ability to program these structures to fold a certain way to carry information and reconfigure themselves means that DNA nanodevices can be designed to do many things. They can, for example, carry drugs and deliver them to targets in clever ways [4], or can be designed to have movable

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parts that can sense and/or amplify signals, or even perform logic functions like a computer. On the other hand, the ability of DNA for charge transfer makes it a suitable candidate for any design of nanoelectronical devices, nanosensors, nanocercuits, and nanowires [5]. Moreover, the spin transport properties of the DNA, as an organic molecule, make it applicable as a spintronic device [6]. Spintronic systems exploit the fact that the electron current is composed of spin-up and spin-down carriers, which carry information encoded in their spin state and interact differently with magnetic materials. Rich physics behind the organic materials and specific functions, such as switchability with light and electrical or magnetic fields, are two important motivations for using the organic materials such as DNA.

In the current study, we have tried to investigate the electron transfer in DNA nanowires by considering the electron spin. We have taken into account the electron-lattice interaction through the Peyrard-Bishop-Holstein (PBH) model by considering the spin degree of freedom. On the other hand, spin-orbit interaction is combined with the PBH model.

2. Materials and methods

We have considered DNA spin-charge lattice with the following Hamiltonian:

$$H = H_{\rm PBH} + H_{\rm so} + H_{\rm Lead}, \tag{1}$$

where $H_{\rm PBH}$ is the Hamiltonian of PBH model for the description of DNA lattice and charge carriers dynamics by considering the spin degree of freedom. $H_{\rm PBH}$ is written as follows [7]:

$$\begin{aligned} H_{\rm PBH} =& \sum_n \left(\frac{1}{2}m\dot{y}_n^2 + V(y_n) + W(y_n, y_{n+1})\right) \\ &+\sum_{n,\sigma}\{\varepsilon_n c_n^{\sigma+}c_n^{\sigma} - V_{n,n+1}(c_n^{\sigma+}c_{n+1}^{\sigma} + c_{n+1}^{\sigma+}c_n^{\sigma}) \\ &+ \chi y_n c_n^{\sigma+}c_n^{\sigma}\}, \end{aligned} \tag{2}$$

where $V(y_n) = D(e^{-ay_n} - 1)^2$ as Morse potential describes the hydrogen binding between the complementary base pairs, $W(y_n, y_{n+1}) = \frac{k}{2}(1 + \rho e^{-b(y_{n+1}+y_n)})(y_{n+1} - y_n)^2$ is the stacking interaction in a DNA chain, $c_n^{\sigma+}(c_n^{\sigma})$ is the creation (annihilation) operator for a spinor with spin σ, $V_{n,n+1}$ is the hopping constant, and χ is the charge-lattice coupling.

$H_{\rm so}$ is the spin-orbit coupling Hamiltonian expressed by the second quantization method as follows:

$$\begin{aligned} H_{\rm so} =& \sum_n \Big[D_{n,n+1}c_n^{\uparrow+}c_{n+1}^{\downarrow} - D_{n,n+1}^{*}c_n^{\downarrow+}c_{n+1}^{\uparrow} \\ &+D_{n-1,n}^{*}c_n^{\downarrow+}c_{n-1}^{\uparrow} - D_{n-1,n}c_n^{\uparrow+}c_{n-1}^{\downarrow}\Big], \end{aligned} \tag{3}$$

where:

$$\begin{aligned} D_{n,n+1} =& it_{\rm so}\sin\theta\{\sin[n\Delta\phi] + \sin[(n+1)\Delta\phi] \\ &+ i\cos[n\Delta\phi] + i\cos[(n+1)\Delta\phi]\}, \end{aligned}$$

and $t_{\rm so}$ is the spin-orbit coupling constant, θ is the twisting angle of DNA, and $\varphi = n\Delta\phi$ is the cylindrical coordinate angle.

$H_{\rm Lead}$ is the Hamiltonian corresponding to the left and right leads written as follows:

$$H_{\rm Lead} = \sum_k \varepsilon_k a_k^{\sigma+}a_k^{\sigma} + t\sum_{k,\sigma}\{a_k^{\sigma+}(c_1^{\sigma} + c_N^{\sigma}) + H.c.\}, \tag{4}$$

where ε_k is the on-site energy of leads, and t is the hopping constant between leads and DNA.

It is clear that the Hamiltonian terms are complex and dealing with them is hard. Then, considering the nonlinear dynamics tools could open a new horizon in understanding the spin transfer mechanism and its effects on DNA. In this way, we have obtained the evolution equations of the system as follows:

$$\begin{aligned} \ddot{y}_n =& \frac{2aD}{m}e^{-ay_n}\left(e^{-ay_n} - 1\right) \\ &+ \frac{kb\rho}{2m}\Big[e^{-b(y_n+y_{n-1})}(y_n - y_{n-1})^2 \\ &+e^{-b(y_{n+1}+y_n)}(y_{n+1} - y_n)^2\Big] \\ &- \frac{\chi}{m}\left(\left|c_n^{\uparrow}\right|^2 + \left|c_n^{\downarrow}\right|^2\right), \end{aligned} \tag{5}$$

$$\begin{aligned} \dot{c}_n^{\uparrow} =& -\frac{i}{\hbar}\Big\{(\varepsilon_n + \chi y_n)c_n^{\uparrow} - V_{n,n+1}\left(c_{n-1}^{\uparrow} + c_{n+1}^{\uparrow}\right) \\ &+D_{n.n+1}c_{n+1}^{\uparrow} - D_{n-1,n}c_{n-1}^{\downarrow}\Big\} + t\sum_{k,n=1}a_k^{\uparrow}, \end{aligned} \tag{6}$$

$$\begin{aligned} \dot{c}_n^{\downarrow} =& -\frac{i}{\hbar}\Big\{(\varepsilon_n + \chi y_n)c_n^{\downarrow} - V_{n,n+1}\left(c_{n-1}^{\downarrow} + c_{n+1}^{\downarrow}\right) \\ &-D_{n,n+1}^{*}c_{n+1}^{\uparrow} + D_{n-1,n}^{*}c_{n-1}^{\uparrow}\Big\} + t\sum_k a_k^{\downarrow}, \end{aligned} \tag{7}$$

$$\dot{a}_k^{\uparrow} = -\frac{i}{\hbar}\left[\varepsilon_k a_k^{\uparrow} + t\left(c_1^{\uparrow} + c_N^{\uparrow}\right)\right], \tag{8}$$

$$\dot{a}_k^{\downarrow} = -\frac{i}{\hbar}\left[\varepsilon_k a_k^{\downarrow} + t\left(c_1^{\downarrow} + c_N^{\downarrow}\right)\right]. \tag{9}$$

3. Results and discussion

For analyzing the spin transfer mechanism in DNA and investigating the affected parameters, we have tried to obtain the electrical current for spin-up and spin-down

electrons, directly from field equations. These currents are written as follows:

$$I^{\uparrow} = \frac{ie}{\hbar}\left\{\sum_n \left[V_{n,n+1}\left(c_n^{\uparrow+}c_{n-1}^{\uparrow} + c_n^{\uparrow+}c_{n+1}^{\uparrow}\right) + D_{n,n+1}c_n^{\uparrow+}c_{n+1}^{\downarrow} - D_{n-1,n}c_n^{\uparrow+}c_{n-1}^{\downarrow}\right] + t\sum_k\left[\left(c_1^{\uparrow+}+c_N^{\uparrow+}\right)a_k^{\uparrow+} - a_k^{\uparrow+}\left(c_1^{\uparrow+}+c_N^{\uparrow+}\right)\right]\right\}, \quad (10)$$

$$I^{\downarrow} = \frac{ie}{\hbar}\left\{\sum_n \left[V_{n,n+1}\left(c_n^{\downarrow+}c_{n-1}^{\downarrow} + c_n^{\downarrow+}c_{n+1}^{\downarrow}\right) - D_{n,n+1}^{*}c_n^{\downarrow+}c_{n+1}^{\downarrow} + D_{n-1,n}^{*}c_n^{\downarrow+}c_{n-1}^{\uparrow}\right] + t\sum_k\left[\left(c_1^{\downarrow+}+c_N^{\downarrow+}\right)a_k^{\downarrow+} - a_k^{\downarrow+}\left(c_1^{\downarrow+}+c_N^{\downarrow+}\right)\right]\right\}. \quad (11)$$

Using the above relations, we could define the net charge (I_c) and the net spin currents; as a result, the spin polarization relation is as follows:

$$I_s = I^{\uparrow} - I^{\downarrow}, \qquad I_c = I^{\uparrow} + I^{\downarrow}, \qquad P = I_s/I_c.$$

In spintronics, the pure spin current plays an important role in information processing, storage and transfer. A pure spin current is the flow of electron spin angular momentum without the flow of electric charge at the same time. Our main aim is the studying of the pure spin current and its affected parameters.

We have tried to examine the effect of an external magnetic field on the formation of the spin currents in DNA (see Figure 1). In this regard, we have defined the external magnetic field Hamiltonian as follows:

$$H_B = -\mu_B B\sum_n \left(c_n^{\uparrow+}c_n^{\uparrow} - c_n^{\downarrow+}c_n^{\downarrow}\right), \quad (12)$$

where μ_B is the Bohr magneton, and B is the magnetic field in the direction of DNA helix axes. This Hamiltonian term modifies $\dot{c}_n^{\uparrow}(\dot{c}_n^{\downarrow})$ by $\frac{i}{\hbar}\mu_B B c_n^{\uparrow}(-\frac{i}{\hbar}\mu_B B c_n^{\downarrow})$.

Figure 1 shows the regions in magnetic field values in which the minimum charge current exists; as a result, the maximum spin current flows through DNA. These regions are the best values for spintronics applications.

For examining the effect of external magnetic field over the time, we have considered the time series of one of the spin currents (spin-up current) versus the variation of external magnetic intensity (see Figure 2).

It is clear in a 3D scheme that in low field values, the spin-up current is almost zero, but after about $B = 0.2$ mT, the current increases in time.

On the other hand, by applying a time variable field with frequency ω, one could obtain the best interval in frequency domain with maximal spin filtering. To this end, we have considered external magnetic field $B = B_0 \cos\omega t$, where B_0 and ω are the field intensity and frequency, respectively.

It is clear in Figure 3 that spin polarization shows the characteristic peaks in certain frequencies. The maximal peak appears in $\omega = 0.7$ THz. By considering this result, one could design an information coder based on zero-one codes for information transfer aims.

We could examine the simultaneous effects of

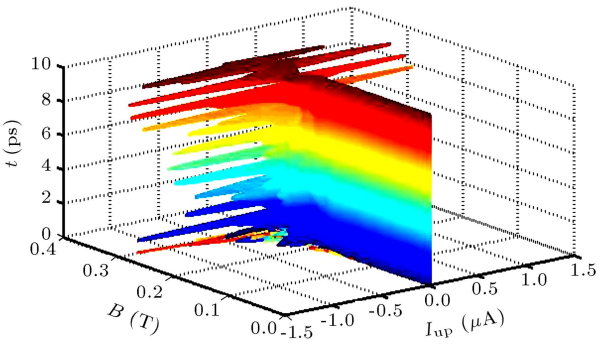

Figure 2. The spin-up time series with respect to the external magnetic field.

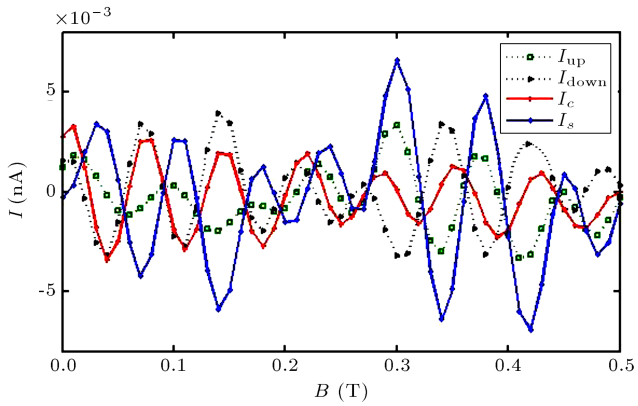

Figure 1. The spin currents with respect to the external magnetic field.

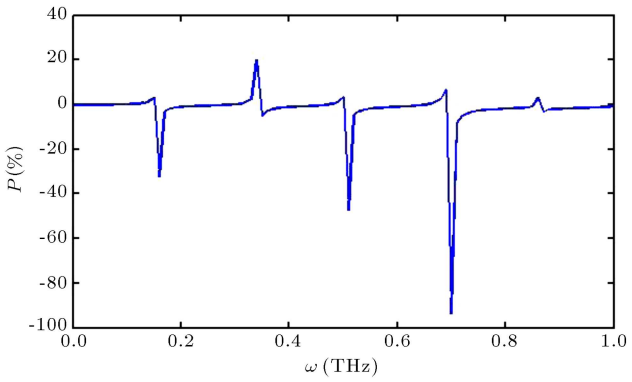

Figure 3. The spin polarization with respect to the frequency of external magnetic field ($B = 0.3$ T).

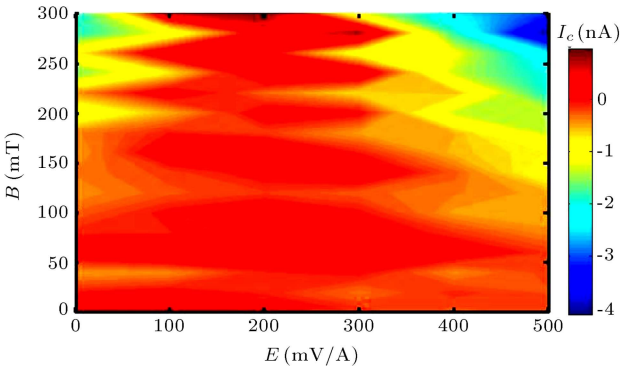

Figure 4. The net spin current with respect to the simultaneous effects of external electrical and magnetic fields.

external electrical and magnetic fields and determine the region in these parameters in which the maximal net spin current flows through DNA. Therefore, we have used the external electrical field Hamiltonian written as follows:

$$H_E = -eEd \sum_{n,\sigma} n c_n^{\sigma +} c_n^{\sigma}, \tag{13}$$

where e is the electron charge, E is the electrical field in helix direction, and d is the distance between the base pairs in the chain. According to the Hamiltonian terms, Eqs. (6) and (7) are modified by $\frac{i}{\hbar} eEndc_n^{\uparrow}$ and $\frac{i}{\hbar} eEndc_n^{\downarrow}$, respectively.

There are the islands in I_c in which the net current is zero; therefore, the maximal spin current flows through DNA (Figure 4).

However, we have studied the effect of the DNA surroundings temperature together with external fields. This work determines the temperatures with which DNA could appear as the maximal spin polarization. In addition, DNA sequence and its length as two influential factors alter the spin polarization of DNA.

4. Conclusions

Organic spintronics combines the spin degree of freedom of electron with its charge for application in nano electronics, information process or transfer. In this regard, DNA as an organic material acts as a spin filter material. We could show a nearly pure spin current through DNA in the presence of external magnetic field. Appling the time variable magnetic field, distinguished among the spin polarization effects in DNA nanowires and used for information coding, can be the innovation of our work. On the other hand, the simultaneous effects of electrical and magnetic fields can determine the pure spin islands in parameters intervals. Therefore, one could choose the best functional regions in parameters values in which DNA plays the role of a spin polarizable nano material. In addition, by considering the DNA wires in different temperatures, we have defined some temperatures as critical ones in which spin polarization has maximum peaks. The simultaneous variations of external fields could specify the intervals with nearly pure spin currents.

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Biographies

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