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Spin filtering Approach in DNA molecules

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Abstract

In this work, we have proposed an analytical approach based on combining of PBH model with spin-orbit coupling interaction and by considering the spin degree of freedom. The following electrical current through DNA corresponding to the spin up and down electrons is directly obtained from the system evolution equations. We could report the SPNDR phenomenon for net spin current in the presence of external electrical field. By applying the electrical and magnetic field, simultaneously, one could determine the regions that the pure spin current is emerged.

Molecular electronics is one of the best candidate in generating the molecular devices. In spite of charge transport, the spin transport in the molecules, as the molecular spintronics, has recently attracted much attention [1]. As compared with conventional semiconductors and metals, the DNA molecule preserves long spin relaxation time which makes it attractive for building spintronic devices and using it to store and process information. In this work, the spin transfer properties of DNA is studied using a combined analytical approach by taking into account the spin degree of freedom and considering the spin-orbit interaction in Peyrard-Bishop-Holstein model [2]. In general, the Hamiltonian of model is written as $H = H_{lat} + H_{car} + H_{\text{int}} + H_{so} + H_{field}$, where H_{lat} is DNA lattice Hamiltonian based on PBD model which has the following form:

$$H_{lat} = \sum_n [\frac{1}{2} m\dot{y}_n^2 + V(y_n) + W(y_n, y_{n+1})] \tag{1}$$

where $V(y_n) = D(e^{-ay_n} - 1)^2$ is the Morse potential and $W(y_n, y_{n+1}) = \frac{k}{2}(1+\rho e^{-b(y_{n+1}+y_n)})(y_{n+1}-y_n)^2$ is the stacking interaction between the adjacent base-pairs.

We could write the electric part of Hamiltonian as follows:

$$H_{car} + H_{\text{int}} = \sum_{n,\sigma} [\varepsilon_n c_n^{\sigma+} c_n^{\sigma} - V_\circ (c_n^{\sigma+} c_{n+1} + c_{n+1}^{\sigma+} c_n^{\sigma})] + \sum_{n,\sigma} \chi y_n c_n^{\sigma+} c_n^{\sigma} \tag{2}$$

that $c_n^{\sigma+} (c_n^{\sigma})$ is the creation (annihilation) operator for an electron with spin σ in n-th site. ε_n is the on-site energy of base-pair, $V_\circ$ hopping constant between the base-pairs in DNA chain and χ is the electron-lattice constant.

Also, the spin-orbit interaction using the creation and annihilation operators in second quantization approach has the following form:

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

Where $D_{n,n+1} = -it_{so} \sin\theta \{\sin[n\Delta\phi] + \sin[(n+1)\Delta\phi] - i\cos[n\Delta\phi] - i\cos[(n+1)\Delta\phi]$, t_{so} is spin-orbit coupling constant, θ is the DNA helix angle and $\phi = n\Delta\phi$ is the twist angle in cylindrical coordinate. On the other hand, the time-reversal relation leads to $D_{n,n-1} = D_{n-1,n}^{*}$.

In this work, the effect of external electrical and magnetic field on spin transport in DNA is studied using the following Hamiltonian [3]:

$$H_{field} = -e\sum_{n,\sigma} dE\cos[(n-1)\Delta\phi] c_n^{\sigma+} c_n^{\sigma} - \sum_n -\mu_B B(c_n^{\uparrow+} c_n^{\uparrow} - c_n^{\downarrow+\downarrow} c_n) \tag{4}$$

where E and B are the electrical and magnetic field intensities, respectively.
In the current study, for studying the spin transfer in DNA and investigating the affected factors on it, we could use the nonlinear dynamical systems theory. Then, we try to derive the system evolution equations from Hamiltonian, transform it to first-order differential equations, and solve it. The motion equations of system is written as following:

$$\ddot{y}_n = \frac{2aD}{m} e^{-ay_n}(e^{-ay_n}-1) + \frac{kb\rho}{2m}[e^{-b(y_n+y_{n-1})}(y_n - y_{n-1})^2 + e^{-b(y_{n+1}+y_n)}(y_{n+1}-y_n)^2] - \frac{\chi}{m}(|c_n^{\uparrow}|^2 + |c_n^{\downarrow}|^2) \tag{5-a}$$

$$\dot{c}_n^{\uparrow} = -\frac{i}{\hbar}\{(\varepsilon_n + \chi y_n - eE\cos[(n-1)\Delta\phi]d - \mu_B B)c_n^{\uparrow} - V_\circ(c_{n-1}^{\uparrow} + c_{n+1}^{\uparrow}) + D_{n,n+1}c_{n+1}^{\downarrow} - D_{n-1,n}c_{n-1}^{\downarrow}\} \tag{5-b}$$

$$\dot{c}_n^{\downarrow} = -\frac{i}{\hbar}\{(\varepsilon_n + \chi y_n - eE\cos[(n-1)\Delta\phi]d + \mu_B B)c_n^{\downarrow} - V_\circ(c_{n-1}^{\downarrow} + c_{n+1}^{\downarrow}) - D_{n,n+1}^{*}c_{n+1}^{\uparrow} + D_{n-1,n}^{*}c_{n-1}^{\uparrow}\} \tag{5-c}$$

For analyzing the spin transfer mechanism in DNA, we have tried to obtain the electrical currents corresponding to spin up and down electrons directly from motion equations. Therefore, we could write:

$$I^{\uparrow} = \frac{ie}{\hbar}\sum_n V_\circ(c_n^{\uparrow+}c_{n-1}^{\uparrow} + c_n^{\uparrow}c_{n+1}^{\uparrow}) + D_{n,n+1}c_n^{\uparrow+}c_{n+1}^{\downarrow} - D_{n-1,n}c_n^{\uparrow+}c_{n-1}^{\downarrow} \tag{6-a}$$

$$I^{\downarrow} = \frac{ie}{\hbar}\sum_n V_\circ(c_n^{\downarrow+}c_{n-1}^{\downarrow} + c_n^{\downarrow}c_{n+1}^{\downarrow}) - D_{n,n+1}^{*}c_n^{\downarrow+}c_{n+1}^{\uparrow} + D_{n-1,n}^{*}c_n^{\downarrow+}c_{n-1}^{\uparrow} \tag{6-b}$$

Different factors affect on the current owing through DNA. Using the nonlinear dynamics methods and obtained equations for the current operators, we could easily assess the effect of various factors such as magnetic and electrical fields on spin transfer in DNA. We could define the spin polarization based on the net charge (I_c) and net spin (I_s) currents. Therefore, the currents and spin polarization (P) could be written as following:

$$I_c = I^{\uparrow} + I^{\downarrow}, \qquad I_s = I^{\uparrow} - I^{\downarrow}, \qquad P = \frac{I^{\uparrow} - I^{\downarrow}}{I^{\uparrow} + I^{\downarrow}} \tag{7}$$

It is worth noting that DNA molecule is a promising candidate for molecular electronics. On the other hand, magnetic and electrical field have considerable effects on spin dependent charge transfer in DNA. In the current study, we have examined the effect of both fields on the spin currents in DNA. The used constants and parameters values is represented in Refs. [2, 4, 5]. By applying a constant magnetic field on DNA molecule, it is found that spin-up and spin-down currents show different behaviors (Fig. 1). By increasing the field intensity, one could apperceive the decreasing in the I_c owing through DNA chain. Therefore, I_c is much less than I_s and could be neglected. Now, it is worth noting that I_s could been used in information transport where the pure spin current is preferred. Then, we try to investigate the spin-selective tunneling of electrons through DNA in the presence of an external electric field. It is remarkable that it will be possible to distinguish between the two spin states. It is shown that the net spin current is more intuitive in the recent conditions (see Fig. 2).

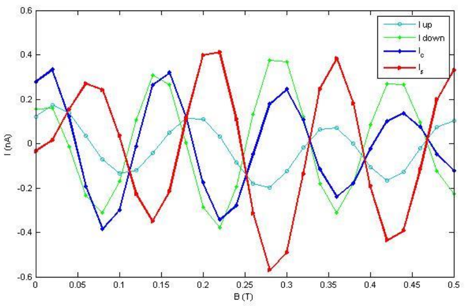

Fig 1: The currents in the presence of magnetic fields.

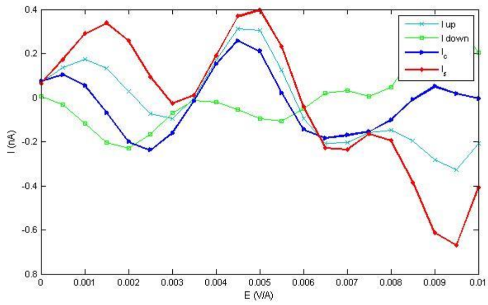

Fig 2: The currents in the presence of electrical fields.

Also, we have study the I-V characteristic diagram for the net spin owing through DNA. There are the regions with negative gradient together with the regions with quasi-linear property in Fig. 3.

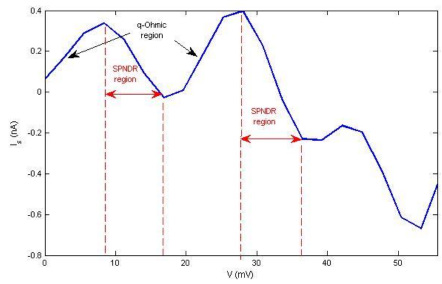

Fig 3: I-V characteristic diagram for I_s current.

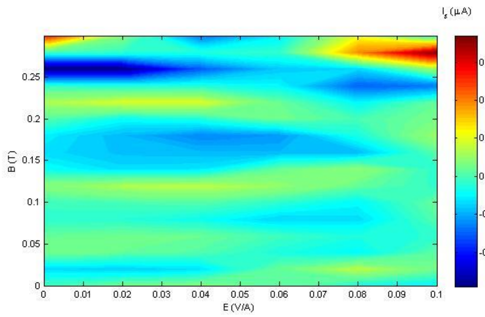

Fig 4: The I_s current in the presence of electrical and magnetic fields, simultaneously.

The negative differential resistance (NDR) has previously reported in DNA molecules [6]. Now, we have reported the spin polarized negative differential resistance (SPNDR) in DNA by studying the I-V characteristic for spin current. This effect is experimentally reported in a self-assembled molecular chain and graphene nanoribbons, previously [7]. A SPNDR device will enrich spintronics as well. The intrinsic and switchable features of the SPNDR effect are therefore important for future spintronic device design.

Also, through the applying the electrical and magnetic field simultaneously, we could see I_s dominate to I_c for certain values of fields and create the pure spin current. It is shown that there are the islands in which I_s is maximal, therefore one could report the pure spin current.

Results

The results based on a combined PBH model show the spin filtering effect for the electron current flows through DNA. The SPNDR effect and polarized current appeared in DNA make it a good candidate in molecular electronics and spintronics. On the other hand, the nearly pure spin current reported in this work could been used in information theory for information process and transfer.

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