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Heat Driven Spin Currents in DNA Chains

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ABSTRACT. Recent discoveries of phenomena involving the interaction of heat currents and spin currents have originated a vigorous field of spintronics, known as spincaloritronics. Meanwhile, creating the spin current via the applying the temperature gradient attracts much attention among the scientists. By using spin polarization, the spintronic phenomenon able to store and process the information, so transporting information is interested. On the other hand, widely known for storage of genetic information in biology, DNA has also been recognized as a useful building material, in the field of nanotechnology. Here, we study the spin-selectivity properties of DNA chains by assuming the Peyrard-Bishop-Holstein model. The temperature gradient applied using the temperature difference between two ends of chain via the Nose-Hoover thermostat. We suppose the generation of net spin currents by heat driving. The effect of external magnetic and electrical fields simultaneously with temperature gradient is studied. The obtained results show the appropriate range of affected factors for creating the spin current. Thus, one can design a most efficient device for spin transport.

Keywords: Spincaloritronics; Spin polarization; Biological systems; Temperature gradient.

INTRODUCTION

Spincaloritronics is the field combining thermoelectrics with spintronics and nanomagnetism.[1] The work of Johnson and Silsbee indicated that, in spintronics and magnetic systems, heat currents can couple to spin currents as well as charge currents.[2] Organic materials are cheap, mechanically flexible, chemically interactive and simple to fabricate.[3] DNA is an important organic biomolecule which is suggested as an organic spin filter.[4] The spin has a number of significant confidants, which make it extremely favorable for transferring and manipulating information.[5] Behnia et al.[6] investigated the effect of the electrical and magnetic field and sequence variation on the spin polarization of DNA earlier.

Here we are attempted to study the temperature gradient effect on the spin polarization of DNA and thus determined the spin caloritronic phenomenon in DNA, firstly. We used the DNA nanowire as organic material for investigating the spin-polarized current via the interaction of the electron spin with heat current. The spin effect is added to PBH Hamiltonian for using in the current study.[7] Charge transfer is modelled through a tight-binding model. In the current study, Hamiltonian and evolution equations are nonlinear and show numerous sensitivity to initial conditions. We have used chaos theory as useful tools to create a new attitude into the spin transport mechanism and its influences on DNA. In this way, we have used modified PBH model and derived the evolution equations from the Hamiltonian system. We have immersed the system in a thermal bath to create a temperature gradient in the system. The bath is formulated through a Nose-Hoover thermostat simulation.

MATERIALS AND METHODS

By assuming of N base-pairs spin-charge-lattice system (as shown in Fig. 1), the following Hamiltonian can be derived:

$$H = H_{lat} + H_{car} + H_{int} + H_{fields} + H_{so} \quad (1)$$

where,

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

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H_{lat} is the lattice Hamiltonian by nonharmonic PBD model.[7] Here, $V(y_n) = D_n(e^{-a_n y_n} - 1)^2$ is the Morse potential and $W(y_n, y_{n+1}) = \frac{k}{2}(1 + \rho e^{-\alpha(y_n + y_{n+1})})(y_{n+1} - y_n)^2$ is the stacking interaction between adjacent base-pairs.

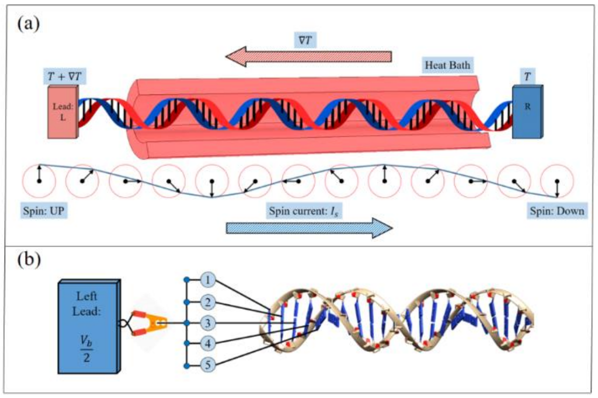

Fig. 1: Outline of the physical model; (a) DNA molecule embedded in the heat bath and connected to electrodes (L & R) in temperature gradient, (b) DNA molecule in the junction: the first five base pairs connected to the electrode (in both ends).

The electronic part of Hamiltonian is given by eq. (3):

$$H_{car} = \sum_{n,\sigma}[\varepsilon_n C_n^{\sigma\dagger} C_n^{\sigma} - V_{n,n+1}(C_n^{\sigma\dagger} C_{n+1}^{\sigma} + C_{n+1}^{\sigma\dagger} C_n^{\sigma})] \quad (3)$$

Where, $C_n^{\sigma\dagger}$ and C_n^{σ} are creation and annihilation operators on n-th site with spin σ, respectively. The on-site energy for base pair in n-th site is called ε_n. In this model, the charge hopping between the nearest neighbor base pairs is given by $V_{n,n+1}$, eq. (4):

$$H_{int} = x \sum_{n,\sigma} y_n C_n^{\sigma\dagger} C_n^{\sigma} \quad (4)$$

H_{int} is the effect of charge lattice interaction, x is the electron-lattice coupling constant, and H_{so} is the spin-orbit interaction.[6]

$$H_{SO} = \sum_n [2it_{so}\cos\theta\,(C_n^{\dagger\uparrow} C_{n+1}^{\uparrow} - C_n^{\dagger\uparrow} C_{n-1}^{\uparrow} - C_n^{\dagger\downarrow} C_{n+1}^{\downarrow} + C_n^{\dagger\downarrow} C_{n-1}^{\downarrow}) + D_{n,n+1} C_n^{\dagger\uparrow} C_{n+1}^{\downarrow} - D_{n,n+1}^{*} C_n^{\dagger\downarrow} C_{n+1}^{\uparrow} + D_{n-1,n}^{*} C_n^{\dagger\downarrow} C_{n-1}^{\uparrow} - D_{n-1,n} C_n^{\dagger\uparrow} C_{n-1}^{\downarrow}] \quad (5)$$

where, $D_{n,n+1} = it_{so}\sin\theta\{\sin[n\Delta\varphi] + \sin[(n+1)\Delta\varphi] + i\cos[n\Delta\varphi] + i\cos[(n+1)\Delta\varphi]\}$, t_{so} spin-orbit interaction constant and θ is the helix angle and $\varphi = n\Delta\varphi$ is the cylindrical coordinate with ϕ the twist angle and $D_{n,n-1} = D_{n-1,n}^{*}$. In the present study. In order to study the influences of external fields on electron spin transfer, the following general Hamiltonian is considered in which H_E and H_B are electrical and magnetic fields, respectively.[7]

$$H_{Fields} = H_E + H_B \quad (6)$$

Where,

$$H_E = -e \sum_{n,\sigma=\uparrow,\downarrow} Ed\cos[(n-1)\Delta\varphi] C_n^{\sigma\dagger} C_n^{\sigma} \quad (7)$$

and,

$$H_B = \sum_n (-\mu_B B C_n^{\uparrow\dagger} C_n^{\uparrow} + \mu_B B C_n^{\downarrow\dagger} C_n^{\downarrow}) \quad (8)$$

$\mu_B = \frac{e\hbar}{2mc} = 5/78838\uparrow\times 10^{-5}$ is the Bohr magneton. We obtain the evolution equations through the Hamilton equations for classical part. Via the Heisenberg approach $\dot{C}_n^{\uparrow\downarrow} = -\frac{i}{\hbar}[C_n^{\uparrow\downarrow}, H]$, we can derive the electronic part equation. We use Nosé's Hoover thermostat [6] which can be formulated by $\dot{\xi} = \frac{1}{M}(\sum_n m\dot{y}^2 - NK_BT)$. ξ is the thermodynamics friction coefficient. T is the temperature applied to the system by the thermal bath and M = 1000 is the constant of Nosé-Hoover thermostat.

RESULTS AND DISCUSSION

As mentioned, we use chaos theory tools to analyze system behavior. In this regard, evolution equations are as follows:

$$\ddot{y}_n = \frac{2a_n D_n}{m} e^{-a_n y_n}(e^{-a_n y_n} - 1) + \frac{\kappa b\rho}{2m}[e^{-b(y_n + y_{n-1})}(y_n - y_{n-1})^2 + e^{-b(y_{n+}y_{n+1})}(y_{n+1} - y_n)^2] - \frac{\kappa}{m}[(1 + \rho e^{-b(y_n + y_{n-1})})(y_n - y_{n-1}) - (1 + \rho e^{-b(y_{n+1} + y_n)})(y_{n+1} - y_n)] - \frac{V_0\beta_n}{m}\left[\begin{array}{l} C_{n-1}^{t\uparrow} C_n^{\uparrow} + C_n^{t\uparrow} C_{n-1}^{\uparrow} - C_n^{t\uparrow} C_{n+1}^{\uparrow} - C_{n+1}^{t\uparrow} C_n^{\uparrow} + C_{n-1}^{t\downarrow} C_n^{\downarrow} + \\ C_n^{t\downarrow} C_{n-1}^{\downarrow} - C_n^{t\downarrow} C_{n+1}^{\downarrow} + C_{n+1}^{t\downarrow} C_n^{\downarrow} \end{array}\right] - \xi \dot{y}_n \quad (9)$$

$$\dot{C}_n^{\uparrow} = \frac{-i}{\hbar}\{(\varepsilon_n + \chi y_n) C_n^{\uparrow} + W_{n-1,n}^{*} C_{n-1}^{\uparrow} + W_{n,n+1} C_{n+1}^{\uparrow} - D_{n,n-1} C_{n-1}^{\downarrow} + D_{n,n+1} C_{n+1}^{\downarrow}\} \quad (10)$$

$$\dot{C}_n^{\downarrow} = \frac{-i}{\hbar}\{(\varepsilon_n + \chi y_n) C_n^{\downarrow} + W_{n-1,n} C_{n-1}^{\downarrow} + W_{n,n+1}^{*} C_{n+1}^{\downarrow} + D_{n-1,n}^{*} C_{n-1}^{\uparrow} - D_{n,n+1}^{*} C_{n+1}^{\uparrow}\} \quad (11)$$

where, $W_{n,n+1} = -V_{n,n+1} + 2it_{so}\cos\theta$.
Spin-up and spin-down currents can be obtained straightforwardly from the field equations using particle density operator in Heisenberg picture. $n_i^{\sigma} = C_i^{\sigma\dagger}C_i^{\sigma}$ is the charge density and $I^{\uparrow\downarrow} = -\frac{ie}{\hbar}[n_i^{\sigma}, H]$. The time-dependent electrical currents are presented as follows:

$$I^{\uparrow}(t) = \frac{-ie}{\hbar}\sum_{n}\{W_{n,n+1}C_n^{\uparrow\dagger}C_{n+1}^{\uparrow} + W^{*}_{n-1,n}C_{n-1}^{\dagger\uparrow}C_n^{\uparrow} + D_{n,n+1}C_n^{\downarrow\dagger}C_{n+1}^{\downarrow} - D_{n-1,n}C_{n-1}^{\dagger\downarrow}C_n^{\downarrow}\} \quad (12)$$

$$I^{\uparrow}(t) = \frac{-ie}{\hbar}\sum_{n}\{W^{*}_{n,n+1}C_n^{\dagger\downarrow}C_{n+1}^{\downarrow} + W_{n-1,n}C_{n-1}^{\dagger\downarrow}C_n^{\downarrow} - D^{*}_{n,n+1}C_n^{\uparrow\dagger}C_{n+1}^{\uparrow} + D^{*}_{n-1,n}C_{n-1}^{\dagger\uparrow}C_n^{\uparrow}\} \quad (13)$$

Using current operator equations, the effects of various factors such as electric and magnetic fields on the system are investigated. Now, by characterizing the net charge, $I_c = I^{\uparrow} + I^{\downarrow}$, and net spin, $I_s = I^{\uparrow} - I^{\downarrow}$, currents, The spin-dependent current is examined in DNA.
Fig. 2 shows time series of spin currents at temperature gradient ΔT = 15 K. It is clear that, due to the temperature gradient, spin up and spin down behave distinctly. The spin up has the maximal values at sometimes, while spin down current is low at all times. Thus, the effect of temperature gradient can be appeared in spin currents.

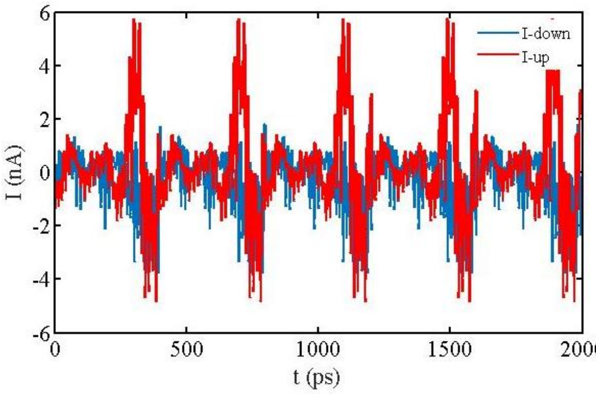

Fig. 2: Spin current time series at ΔT = 15 K.

It is significant that the DNA molecule is a good candidate for sub-atomic gadgets. Further, the gate voltage influences the spin transport of DNA atoms. It is shown that the variation of the electrical field creates the polarized currents (Fig. 3). At low fields, spin polarization is low. But, when the range of field approaches to E = 3 mV/A, spin current starts to increase. The spin current approaches to maximal value, when the field is about E= 3.5 mV/A. This result is obtained at ΔT = 25 K. Therefore, the effect of the external gating is represented clearly.

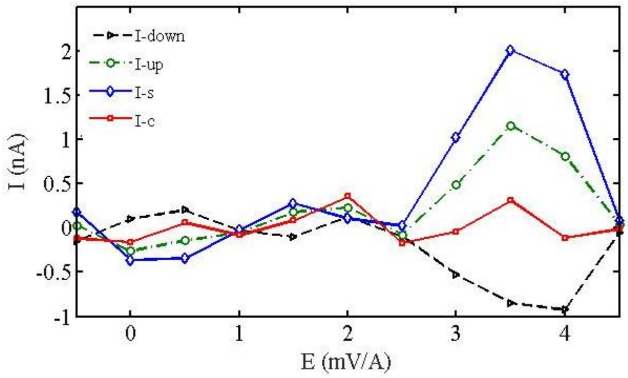

Fig. 3: Spin currents with respect to external electrical field at ΔT = 25 K.

Since the magnetic field has notable influences on spin-dependent charge transfer in DNA, we investigated that's effect. The spin-up current approaches to zero, whiles spin-down current get high values in some fields, Fig. 4. This result can verify the efficacy of magnetic field on the spin polarization in DNA. The external field and temperature gradient applied simultaneously to DNA. In the absence of temperature gradient, the spin polarization phenomenon is lighter.

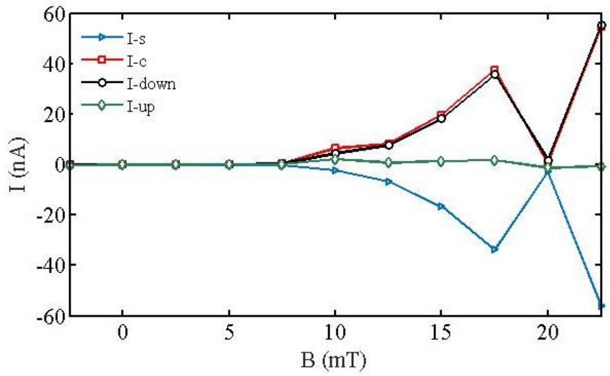

Fig. 4: Spin currents as for the external magnetic field at ΔT = 25 K.

Therefore, the simultaneous study of temperature gradient and external electrical or magnetic field shows creating the temperature gradient dependent spin current in DNA chains.

CONCLUSION

Spin caloritronics is an emerging field at the boundary between thermal transport phenomena and spin physics. The greater part of the advancement in this new innovation is right now dependent on inorganic materials. Organic electronics is discovering its place as a significant innovation for creation of different nanoelectronic gadgets. In this regard, we have tried to study the spin current created via the applied temperature gradient in DNA chain. The temperature gradient is applied to the system via the temperature difference between two ends of the chain. Due to such temperature difference system goes to create the polarized spin current. This phenomenon is examined in presence of external electrical and magnetic fields. Based on the results, it is shown that each of them is the effective factor for spin polarization. Thus, one can choose the most appropriate range of applied fields or temperature gradient for designing the spin caloritronic devices.

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