Electrically Driven Spin Currents in DNA

Dhurba Rai and Michael Galperin

Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA

Abstract

We study the generation of pure spin currents (spin pumping) by electric field driving in a simple two-level bridge model. This scheme is then applied to study spin transport in single stranded (ss) and double stranded (ds) DNA junctions. We show the possibility of generating pure spin currents in DNA, even in the absence of spin-orbit coupling. Generating spin polarized current is easier than generating pure spin current, the latter requires some extra efforts (suitable electric gating and low temperature).

Model and Method

Model Hamiltonian

$$\hat{H} = \hat{H}_M(t) + \sum_{K=L,R}(\hat{H}_K + \hat{V}_K) \qquad (1)$$

$$\hat{H}_M(t) = \sum_{b=1}^{N_b}\sum_{\sigma,\sigma'}\Big(\sum_{m=1}^{N}(\varepsilon^{(b)}_{m,\sigma\sigma'}(t)\hat{d}^{(b)\dagger}_{m\sigma}\hat{d}^{(b)}_{m\sigma'} + \delta_{N_b,2}\delta_{\sigma,\sigma'}\, t_m^{(b\bar{b})}\hat{d}^{(b)\dagger}_{m\sigma}\hat{d}^{(b)}_{m\sigma})$$

$$+\sum_{m=1}^{N-1}[(\delta_{\sigma,\sigma'}t^{(b)}_{m,m+1} + it_{so}[\sigma^{(b)}_{\sigma\sigma'} + \sigma^{(b)}_{m+1,\sigma\sigma'}])\,\hat{d}^{(b)\dagger}_{m\sigma}\hat{d}^{(b)}_{m+1\sigma'} + H.c.]\Big) \qquad (2)$$

$$\hat{H}_K = \sum_{k=K;\sigma}\varepsilon_k \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} \quad and \quad \hat{V}_K = \sum_{b=1}^{N_b}\sum_{k=K;\sigma}(\mathrm{V}^{(b)}_{mk}\hat{d}^{(b)\dagger}_{m\sigma}\hat{c}_{k\sigma} + H.c.) \qquad (3)$$

where the notation have usual meanings. The on-site energy of site m on bridge b is

$$\varepsilon^{(b)}_{m,\sigma\sigma'}(t) = \delta_{\sigma,\sigma'}\,[\varepsilon^{(b)} - (\vec{\mu}^{(b)}_m \cdot \vec{E}(t))] - \mu_{\mathrm{B}}(\vec{\sigma}_{\sigma\sigma'}\cdot\vec{B}) \qquad (4)$$

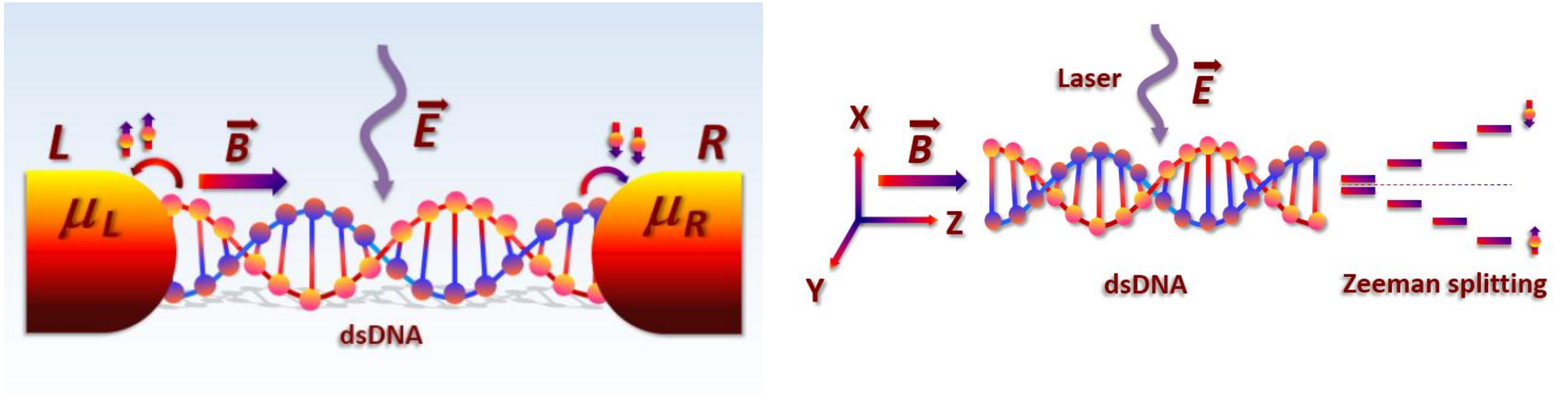

Fig. 1. Sketches of the molecular systems (DNA and molecular bridge) coupled to metal leads (*L*,*R*) under driving by dc magnetic field, $\vec{B}$, and ac electric, $\vec{E}(t)$, fields.

Parameters Used

$\vec{B}(\vec{r}) = (-xk/2, -yk/2, zk)$ (nonuniform), $\vec{B} = (0,0,B)$ (uniform), $k = 8\,\mathrm{mT/nm}$(field gradient), $B = 500\,\mathrm{mT}$.

Harmonic driving : $E(t) = E_0\cos(\omega t)$, Harmonic mixing : $E(t) = E_0\cos(\omega t) + (E_0/2)\cos(2\omega t + \varphi)$.

$\varphi = \pi/4, \omega = 0.1\,\mathrm{eV}, T = 300\mathrm{K}, \Gamma_L = \Gamma_R = 0.05\,\mathrm{eV}, E_{\mathrm{F}} = 0, n = 20$.

Method: Floquet theory + NEGF

Harmonically driven junction, Eqs. (1) to (3) is treated within the Floquet theory combined with nonequilibrium Green's function formalism [G. Stefanucci et. al. Phys. Rev. B 77, 075339 (2008)]. The retarded Green function can be expended as

$$G^r(t,t') = \sum_{n=-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{dE}{2\pi}G^r_n(E)\,e^{-iE(t-t')+in\omega t'} \qquad (5)$$

where ω is the fundamental frequency and n is the Floquet index. The coefficients of expansion $G_n(E) \equiv G^r_n(E-n\omega) = [G^a_{-n}(E-n\omega)]^\dagger$ satisfy recurrence relations

$$G_n(E) \equiv G^{(0)}_n(E)\,[\delta_{n,0} + \sum_{n'=-\infty}^{+\infty}\mathrm{U}_{n'}\mathrm{G}_{n-n'}(E)] \qquad (6)$$

where $G^{(0)}_n(E)$ is the retarded Green function of the system in absence of driving. Self energy in a wide-band limit, $\left(\Sigma^r_K(E)\right)_{bm\sigma,b'm'\sigma'} \equiv -i\delta_{\sigma,\sigma'}\Gamma^K_{bmb'm'}/2$. In Eq. (6) U_n couples different Floquet indices, $\mathrm{U}_n = -\delta_{n,\pm1}\,\mu_M E_0/2$ (monochromatic driving) $\mathrm{U}_n = -\mu_M E_0\,(\delta_{n,\pm1} + \delta_{n,\pm2}e^{2i\varphi/n}\,/2)/2$ (harmonic mixing). Solving Eq. (6), the dc current can be obtained from

$$I^{\mathrm{dc}}_K = -2\,\mathrm{Re}\int\frac{dE}{2\pi}Tr[G_0(E)\Sigma^<_K(E) + \sum_n G_n(E)\,(\Sigma^<_L(E) + \Sigma^<_R(E))G^\dagger_n(E)\,\Sigma^a_K(E)] \qquad (7)$$

Resolving the spin components, the charge and spin currents are evaluated as

$$I^{\mathrm{dc}}_C = I^{\mathrm{dc}}_\uparrow + I^{\mathrm{dc}}_\downarrow \quad \text{and} \quad I^{\mathrm{dc}}_S = I^{\mathrm{dc}}_\uparrow - I^{\mathrm{dc}}_\downarrow \qquad (8)$$

Parameters Used

$\mathrm{Two-site}: N_{\mathrm{b}} = 1, N = 2, \varepsilon^{(1)} = 0, t^{(1)} = 0.1\,\mathrm{eV}$, distance between the sites=7nm.

$\mathrm{ssDNA}: N_{\mathrm{b}} = 1, N = 10, \varepsilon^{(1)} = 0, t^{(1)} = 0.12\,\mathrm{eV}, t_{so} = 0.01\,\mathrm{eV}$, distance between the sites along helix=0.56nm, and the separation along z axis is 0.34nm, [Guo and Sun, Phys. Rev. Lett. 108, 218102 (2012)].

$\mathrm{dsDNA}: N_{\mathrm{b}} = 2, N = 10, \varepsilon^{(1)}, \varepsilon^{(2)} = 0, 0.3\,\mathrm{eV}, t^{(1)}, t^{(2)} = 0.12\,\mathrm{eV}, -0.1\,\mathrm{eV}, t^{(12)} = -0.3\,\mathrm{eV}$.

Results

I. Two-level bridge

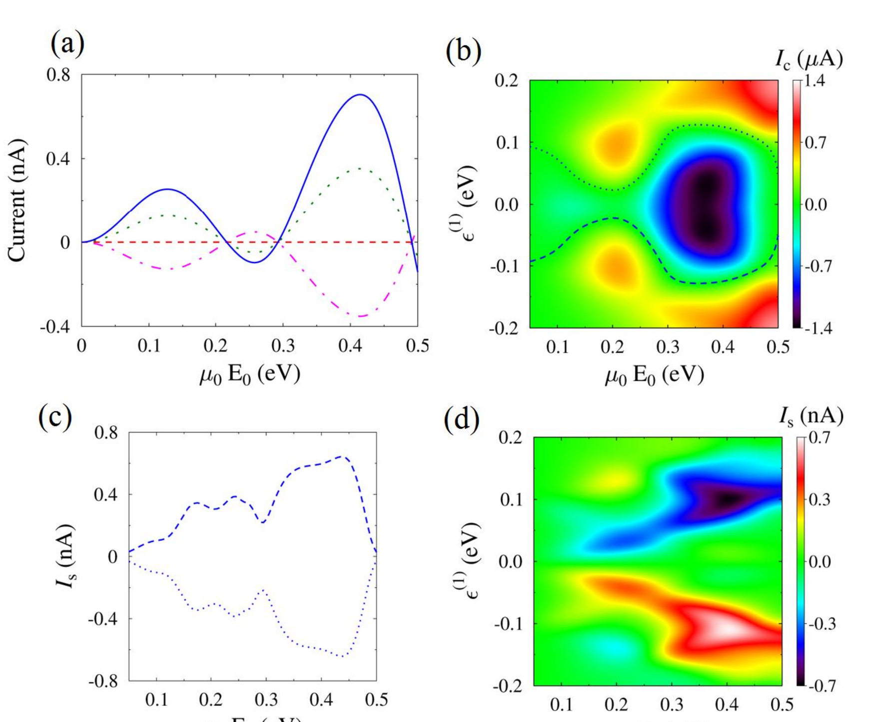

Fig. 2. (a) Two-level bridge under monochromatic driving. (b) Two-level bridge under driving by harmonic mixing. Map of charge current vs. level position and driving amplitude. (c) Pure spin current along the indicated dash and dot paths. (d) Map of pure spin current. In (a), charge current is in dash-red, pure spin current in solid-blue, polarized currents: spin up in dotted-green and spin down in dash-dotted-magenta.

II. Single stranded DNA

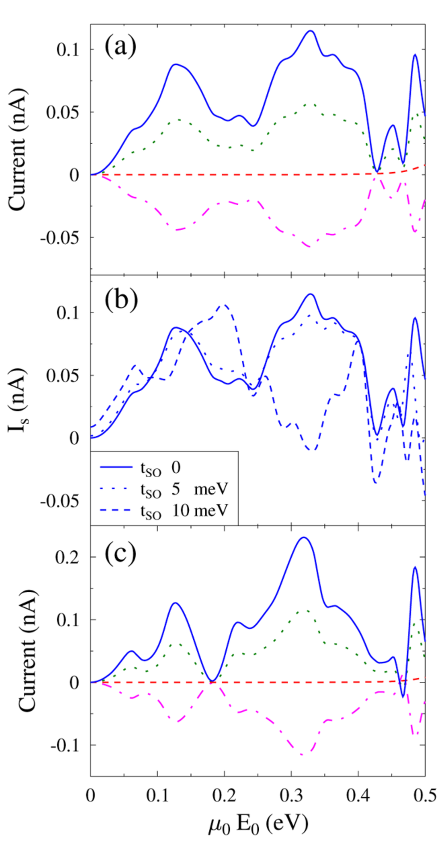

Fig. 3. Monochromatic driving. Currents in (a, b) nonuniform and (c) uniform magnetic field. In (a, c), spin orbit coupling, tso=0.

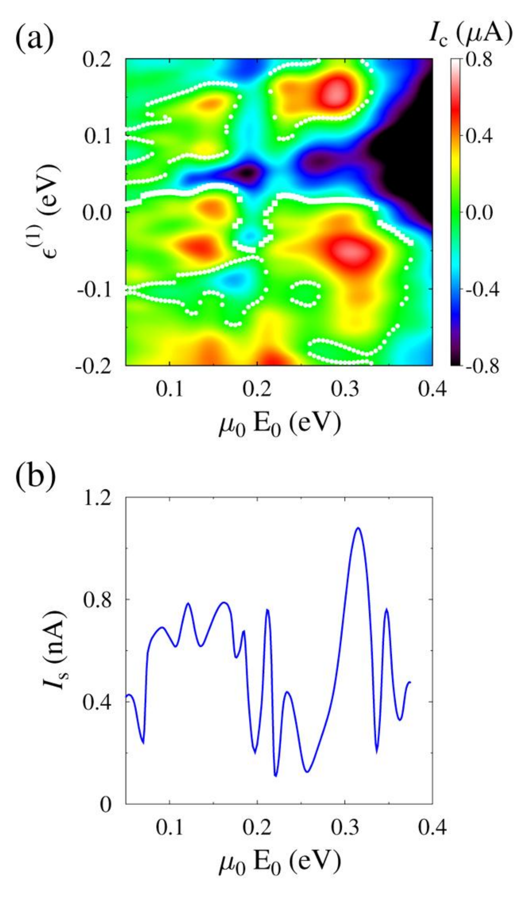

Fig. 4. Driving by harmonic mixing. (a) Map of charge current vs. level position and driving amplitude. (b) Pure spin current along the indicated path (squares). Spin orbit coupling, tso=0 and T=0.5K

III. Double stranded DNA

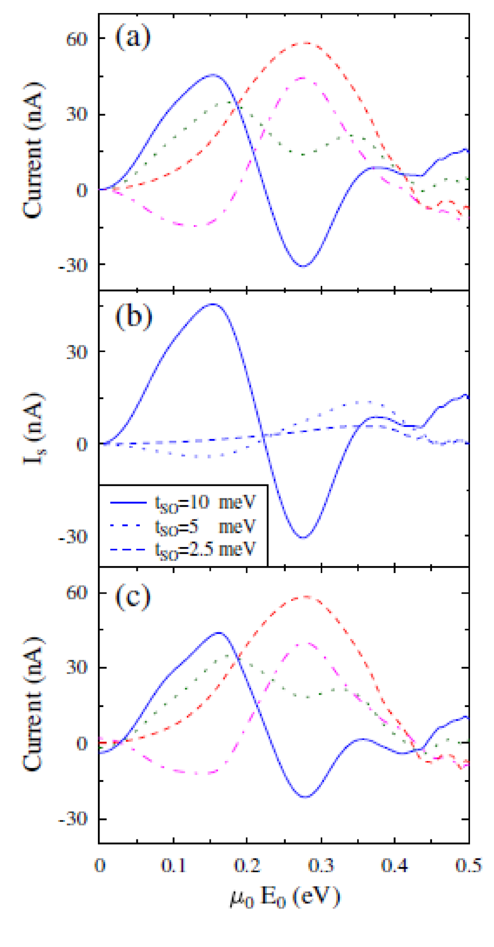

Fig. 5. Monochromatic driving. Currents in (a, b) nonuniform and (c) uniform magnetic field (5T) in presence of spin-orbit interaction.

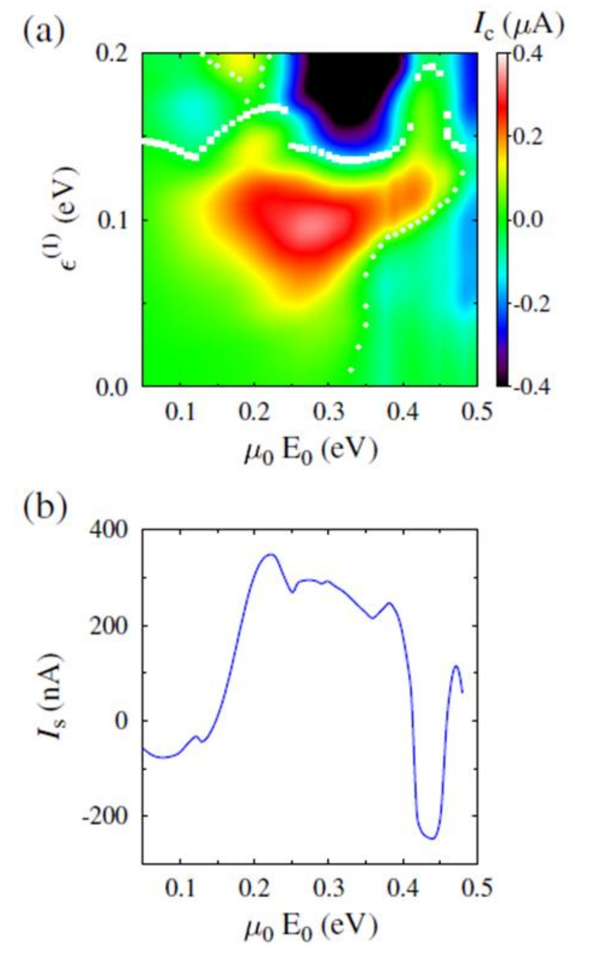

Fig. 6. dsDNA under driving by harmonic mixing. (a) Map of charge current vs. level position and driving amplitude. (b) Pure spin current along the indicated path (white squares). B=0 and T=0.5K

Conclusion

1. It is possible to drive pure spin current in a linear molecular bridge with nonuniform (with driving by monochromatic electric field) or uniform (with electric driving by harmonic mixing) magnetic field.

2 Monochromatic electric field driving is capable of producing pure spin currents on the order of 0.1 nA in ssDNA and 10 nA in dsDNA junctions.

3. Driving by harmonic mixing yields pure spin currents only at very low temperatures and under electric gating conditions in both ssDNA and dsDNA. At room temperature and in absence of gating, spin-polarized currents will be generated.

4. It is the helical structure of DNA that allows the generation of pure spin currents by harmonic driving in the presence of uniform field. This is in sharp contrast with linear bridge molecule wherein symmetry considerations prohibit pumping.

5. In ssDNA, spin-orbit interaction plays only a marginal role in spin pumping in the junction, whereas, in dsDNA, spin-orbit interaction plays the main role.

Acknowledgments

We gratefully acknowledge support from the National Science Foundation (CHE-1057930) and the US-Israel Binational Science Foundation (Grant No. 2008282).