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Model of a gate-controlled spin filter based on a polymer coupled to a quantum wire

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A spin filter based on an organic polymer coupled to a quantum wire is proposed. The spin polarization of the conductance is manipulated by the gate voltage but not by the external magnetic field as in previous spin filters. The results show that a class of organic polymers with spin-polarized flatband can be candidates of the device. The necessary conditions for the fully polarized conductance are discussed. As an application of the result, the device can be used to detect the magnetic transition in the polymer.

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I. INTRODUCTION

The fundamental requirements of any applications based on spintronics include generating spin-polarized currents. Electrical spin injection from metallic or semiconductor ferromagnetic contacts is a traditional method to generate spin-polarized carrier.[1] Quantum-dot (QD) setup is an alternative candidate as a spin filter. Recher *et al.*[2] proposed that a QD in the Coulomb blockade regime weakly coupled to leads acts as a spin filter in an external magnetic field. This kind of spin filter was demonstrated experimentally by Hanson *et al.*[3] through a few-electron QD defined in a two-dimensional electron gas. In the presence of sizable Zeeman splitting, a spin-polarized current can be generated through a QD driven by radio frequency gate voltages.[4,5] The interplay between coherent spin-flip dynamics and Coulomb interaction on a central island with nanometer size also promotes spin-dependent tunneling.[6] Recently, spin battery and spin filter by using ac-driven double QDs have also been proposed.[7,8] The above QD spin filters have following basic characteristics: (i) the chemical potential in the leads or/and the localized levels in the QDs are spin dependent through Zeeman splitting and (ii) there are just few single-electron levels on QDs. Because it is more convenient to control the gate voltage than an external magnetic field, in this paper, we propose a spin filter in which the chemical potential in the leads are not spin dependent and the spin-polarized current is controlled by the gate voltage and not by the external magnetic field.

Recently, electronic components based on molecules have attracted considerable attention. The single-electron transistors made from organic molecule have been experimentally realized.[9] Organic molecules provide powerful systems in this field because the spin and orbital degrees of freedom can be controlled through well defined chemistry. Our device consists of a noninteraction wire with a side-coupled organic polymer *poly*-BIPO.[10] The simplified structure is schematically shown in Fig. 1. The main zigzag chain consists of carbon atoms with a conjugated π orbital. R denotes side radical with nonbonding orbital. This polymer has been described by the Hubbard model in previous works.[11] Due to the existence of a spin-polarized flatband below the gap, the ground state is ferrimagnetic at half-filling. The underlying physics of the spin filter is as follows. With variation of the gate voltage V_g, the chemical potential of the polymer is changed. Hence, the charge and spin in the polymer are tuned by V_g. The spin degeneracy can be lifted by a very small magnetic field applied to the polymer. Because the density of state (DOS) of the polymer is spin polarized, the local DOS at the site 0 of the wire is also polarized by the coupling between site 0 and site C. Therefore, the spin polarized current is controlled by the gate voltage. Our results propose a possibility to design a spin filter through a class of organic polymer[12] and magnetic nanographite[13] that exhibit flatband ferromagnetism.

II. THE MODEL AND COMPUTATIONAL METHOD

In the system shown in Fig. 1, the polymer is described by a Hubbard model and the quantum wire is represented by the nearest-neighbor tight-binding Hamiltonian. A hopping term denotes the link between site C of the polymer and site 0 of the wire. The total Hamiltonian for the one-dimensional quantum wire with a side-coupled polymer can be written as

$$H=-t_0\sum_i (c^\dagger_{i\sigma}c_{i+1\sigma}+\mathrm{H.c.})-\sum_{\langle ij\rangle,\sigma} t_{ij}(p^\dagger_{i,\sigma}p_{j,\sigma}+\mathrm{H.c.})+\sum_{i,\sigma}\epsilon_i n_{pi\sigma}+\sum_i U_i n_{pi\uparrow}n_{pi\downarrow}-t'\sum_{l,\sigma}(c^\dagger_{0\sigma}p_{c\sigma}+\mathrm{H.c.}),\qquad(1)$$

where t_0 is the nearest-neighbor (NN) hopping within the wire. t_{ij} is the NN hopping within the polymer. We assume that the hopping between the NN carbon atoms is t_1, the hopping between the carbon atom and the side radical R is t_2. ϵ_i labels the orbital energy in the polymer. $\epsilon_i=V_g$ and $\epsilon+V_g$ if i denotes the carbon atom and radical R, respectively. $U_i=U_1$ and U_2 denote the on-site Coulomb interaction on carbon atom and radical R, respectively. t' labels the hopping

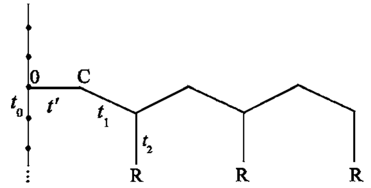

FIG. 1. A schematic system of the quantum wire side coupled to an organic polymer.

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between the site C in the polymer and the site 0 in the wire.

To observe the spin filtering effect, we calculate the zero-bias conductance G_σ for spin σ. At zero temperature and in linear response, the conductance G_σ can be written in the Landauer formula[14]

$$G_\sigma = \frac{e^2}{h} 4\pi^2 [\rho(\epsilon_f)]^2 |t_0^2 G_{00,\sigma}|^2, \tag{2}$$

where $G_{00,\sigma}$ is the Green function with spin σ at the site 0 within the wire, $\rho(\epsilon_f)$ is the DOS of the wire at the Fermi level at the first neighbors of site 0. We use the cluster perturbation theory[15] (CPT) to calculate the Green function of the system. The full system is divided into two parts: the polymer and the wire. The Green function of the full system satisfy a Dyson equation

$$\hat{G} = \hat{g} + \hat{g}\hat{T}\hat{G}, \tag{3}$$

where $\hat{g}$ is the Green function of isolated polymer or the wire. $\hat{T}$ is the hopping matrix between the polymer and the wire. The Green function $\hat{g}$ of the isolated polymer can be calculated by the exact diagonalization (ED).[16] As discussed in Ref. 13, the Green function $\hat{G}$ is exact in the absence of an interaction. When the interactions are turned on, $\hat{G}$ is no longer exact. However, the strong interactions are important mainly for the short-range correlation, which are well treated here by ED within the polymer cluster. To obtain the consistent charge of the polymer, we calculate $\hat{g}$ of the polymer as a combination of the Green function of N and $N+1$ electrons with weight $1-p$ and p,

$$\hat{g} = (1-p)\hat{g}_N + p\hat{g}_{N+1}. \tag{4}$$

The charge of the polymer is[17]

$$q_c = (1-p)N + p(N+1), \tag{5}$$

which can be also expressed as

$$q_c = q_{c,\uparrow} + q_{c,\downarrow}, \tag{6}$$

$$q_{c,\sigma} = -\frac{1}{\pi}\int_{-\infty}^{\epsilon_f} \mathrm{Im}\, G_{ii,\sigma}(\omega) d\omega, \tag{7}$$

where i runs over all the polymer sites. The quantities q_c, N and p can be obtained by resolving Eqs. (3)–(7) self-consistently. The total spin S of the polymer is

$$S = \frac{1}{2}(q_{c,\uparrow} - q_{c,\downarrow}). \tag{8}$$

The spin polarization of the conductance is defined as

$$P_g = \frac{G_\downarrow - G_\uparrow}{G_\downarrow + G_\uparrow}. \tag{9}$$

III. RESULTS AND DISCUSSION

In the following calculation, we take the NN hoping t_0 within the wire as energy unit. The wire is half-filled and the Fermi level is at $\epsilon_f=0$. Because there are no reliable experimental data for the parameters of the polymer, we assume $t_1=1$ and $U_1=1.5$, which is similar to the case of polyacetylene $1.25 < U_1/t_1 < 2$.[18] In the polymer *poly*-BPO, the radical R can be controlled by chemical methods. Our focus is to choose appropriate radical so that the spin-polarized conductance can be produced by controlling the gate voltage. Hence, we stress the effects of the hopping t_2 and the orbital energy ϵ on the conductance. For simplicity, we assume the on-site Coulomb repulsion $U_2=3.0$ at the radical sites, the coupling hopping $t'=0.5$ between the wire and the polymer. As discussed later, the basic physics does not dependent on a specific U_2.

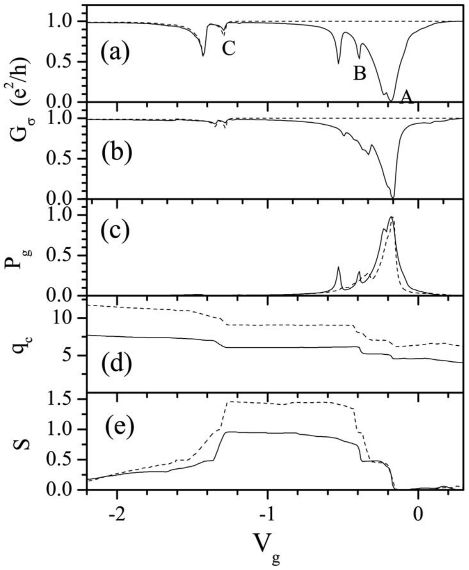

FIG. 2. (a), (b) Conductance G_σ with up-spin (solid line) and down-spin (dashed line) vs gate potential V_g for the polymer size $L=6$ and 9, respectively. (c)–(e) Spin polarization of conductance P_g, charge q_c and total spin S in the polymer for $L=6$ (solid line) and $L=9$ (dashed line). Letters A, B, C in (a) label the point at which the fifth, sixth, and seventh electron enters into the polymer, respectively. Other parameters are $t_1=1$, $t_2=2$, $t'=0.5$, $\epsilon=-0.4$, $U_1=1.5$, and $U_2=3$.

The conductance G_σ is shown in Fig. 2(a) for $t_2=2.0$, $\epsilon=-0.4$ and the polymer size $L=6$. When a positive gate voltage V_g is applied, Figs. 2(d) and 2(e) show that the charge q_c of the polymer is small and the total spin is zero. The conductance in the wire is still e^2/h and is nearly not affected by the polymer. As V_g decreases, the charge q_c increases. At $V_g=-0.18$, the fifth electron enters into the polymer and the total spin is $S=0.5$. The conductance $G_\uparrow$ with up spin decreases continuously and nearly vanishes at this point while $G_\downarrow$ is still e^2/h. Figure 2(c) shows that a fully spin-polarized conductance is obtained by varying the gate voltage. This indicates the device can be used as a spin filter. As V_g continues to decrease, more electrons enter into the polymer while other valleys of the conductance appear. The total spin reaches to the maximum $S=1.0$ at half-filling $q_c=6.0$.

To understand how the electrons enter into the polymer, let us analyze the electrochemical potential of the polymer. We define the electrochemical potential of the polymer as

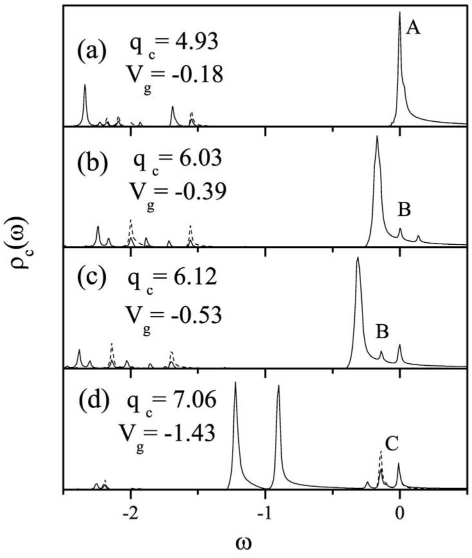

FIG. 3. Local DOS $\rho_c(\omega)$ at cite C of the polymer for different V_g and $L=6$. Other parameters are the same as in Fig. 2. Solid lines and dashed lines correspond to up-spin and down-spin, respectively.

$\mu_{N+1}=E(N+1)-E(N)$, where $E(N)$ is the ground-state energy of the isolated polymer with N electrons. We find $\mu_5\approx 0.18$, which means that the fifth electron enters into the polymer at the point $V_g=-0.18$ since the Fermi level is $\epsilon_f=0$. At this point, the valley A of the conductance $G_\uparrow$ in Fig. 2(a) forms. Similarly, $-\mu_6$ and $-\mu_7$ correspond to the valleys B and C in Fig. 2(a), respectively. Therefore, the conductance valleys exhibits the behavior of Coulomb oscillation. Because there is a Hubbard gap in the middle of the energy band of the polymer [see Fig. 4(a)], the energy difference $\mu_7-\mu_6$ is much greater than $\mu_6-\mu_5$.

It is interesting to note that although the total spin has the maximum $S=1.0$ at half-filling, the spin polarization of the conductance reaches to the maximum at $q_c=5.0$ but not at half-filling $q_c=6.0$. According to the Dyson equation, the Green function $G_{00,\sigma}$ in Eq. (2) is mainly affected by the Green function at site C in the polymer. As a result, the conductance will strongly depends on the local DOS at site C. The DOS $\rho_c(\omega)$ at site C is shown in Fig. 3 for different V_g. The peaks of the DOS close to the Fermi level $\omega=0$ correspond to the valleys of the conductance labeled by the same letter in Fig. 2(a). For $V_g=-0.18$, the charge is $q_c\approx 5.0$ and there is a high peak of the DOS with up spin at the Fermi level $\omega=0$. Accordingly, the conductance $G_\uparrow$ nearly vanishes at this point A. For $V_g=-0.39$, the polymer is nearly half-filled. There is just a small peak of the DOS at the Fermi level although the spin has the maximum $S=1.0$. Hence, a shallow valley of $G_\uparrow$ appears at point B. For $V_g=-1.43$ and $q_c\approx 7.0$, the polarizations in the DOS is very small so that the conductance valley C is nearly not polarized. In the model for a quantum wire side coupled to a single QD, using Friedel's sum rule Aligia *et al.*[19] also obtain the similar result that the maximum of the DOS at QD corresponds to the minimum of the conductance. In the presence of sizable Zeeman splitting, the spin filter based on this single QD is also proposed.[20] Here, we stress that our spin filtering effect is manipulated by the gate voltage and not by Zeeman splitting.

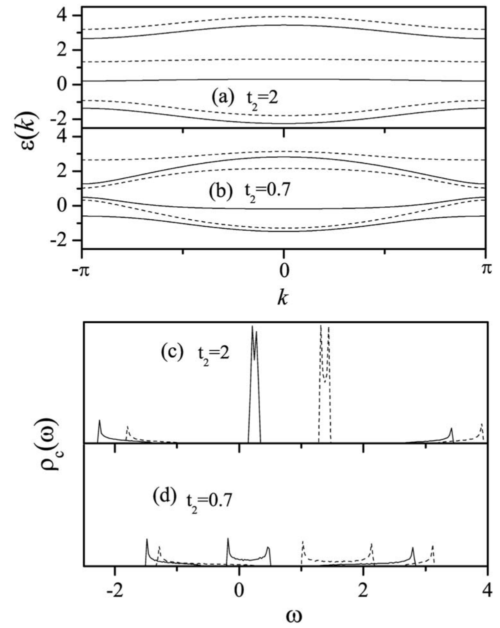

FIG. 4. Energy band $\epsilon(k)$ and local DOS $\rho_c(\omega)$ at site C of an isolated polymer for $t_2=2$ and 0.7. Other parameters are the same as in Fig. 2. Solid lines and dashed lines correspond to up-spin and down-spin, respectively.

In order to investigate the effect of the length of the polymer on the spin filter, Fig. 2(b) shows the conductance for the polymer size $L=9$. As V_g decreases to -0.17, the seventh electron enters into the polymer and the conductance $G_\uparrow$ approaches to zero. Although the quantitative behavior of the conductance is different from that for $L=6$, the tendency for the two cases is similar. At half-filling, the total spin also reaches its maximum $S=1.5$. From the above discussion, one can find that a strongly polarized local DOS at site C is the basis of the spin filtering. To analyze why this local DOS can be realized, the energy band and the local DOS at site C are calculated by the Hartree-Fock approximation[21] (HFA) for the isolated polymer. Figures 4(a) and 4(c) show the results for the same parameters as in Fig. 2. As the filling $n=N/2L$ is larger than $\frac{1}{3}$, the electrons will occupy the flatband with up spin, which corresponds to an abrupt DOS peak just below the middle gap. For $L=6$, when the fifth electron enters into the polymer, the filling satisfies $n>\frac{1}{3}$ and there is a large local DOS at site C. Because the many-body effect is considered more appropriately by the CPT than by the HFA, the abrupt peak of the DOS is widened by the Hubbard repulsion in Fig. 3. As a result, the DOS at the Fermi level is larger for the charge $q_c=5$ than for $q_c=6$. For $L=9$, the filling $n>\frac{1}{3}$ requires the number of the electrons $N\geqslant 7$ so that the polarized conductance appears for $N\geqslant 7$. Therefore, the spin-polarized conductance results from the existence of a spin-polarized flatband in this kind of polymer. Here we have proposed a possibility to design a spin filter through a class of organic polymer[12] and magnetic nanographite[13] that exhibit flatband ferromagnetism.

The hopping t_2 between the carbon atom and the radical may affect the polarization of the conductance. Figure 5

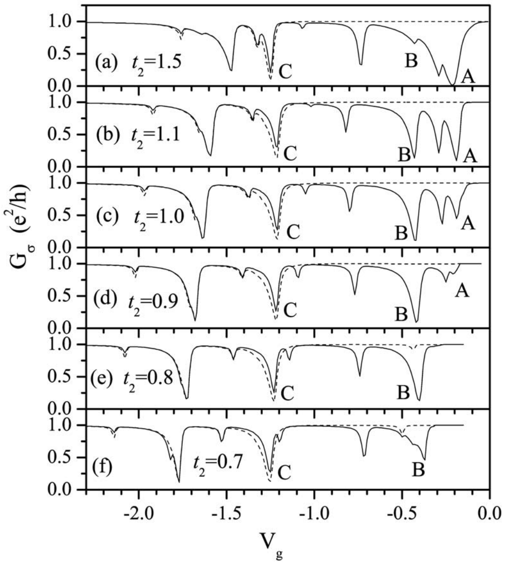

FIG. 5. Conductance G_σ with up-spin (solid line) and down-spin (dashed line) vs gate potential V_g for $L=6$ and different t_2. Other parameters are the same as in Fig. 2.

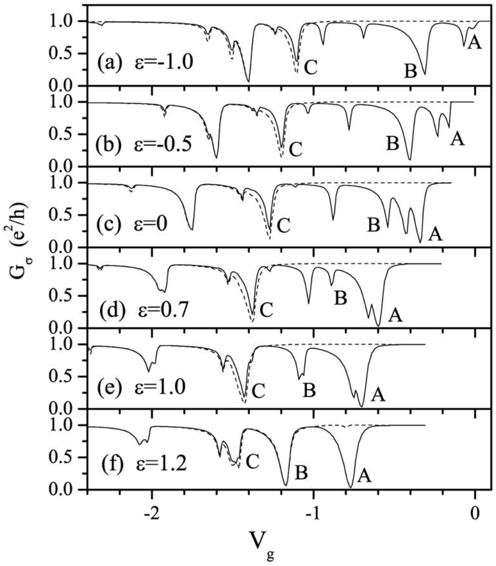

FIG. 7. Conductance G_σ with up-spin (solid line) and down-spin (dashed line) vs gate potential V_g for $L=6$, $t_2=1.0$ and different ϵ. Other parameters are the same as in Fig. 2.

shows this result. As t_2 decreases, the valley A becomes shallow while the depth of valley B increases. For $t_2 \leqslant 0.7$, the valley A disappears while the depth of B also decreases. This behavior of the conductance originates from the variances of the local DOS at site C in the polymer. Figure 6 shows the DOS at site C for different t_2 and V_g. For $t_2=1.5$ and $V_g=-0.21$, there is a high peak with up-spin near the Fermi level $\omega=0$ so that there is a deep valley of conductance $G_\uparrow$ at point A in Fig. 5(a). For the same reason, the small peak B in Fig. 6(b) corresponds to the small valley B in Fig. 5(a). As t_2 decreases to 1.0, the DOS peak A in Fig. 6(c) drops while the peak B in Fig. 6(d) rises so that in Fig. 5(c), the conductance $G_\uparrow$ at point A increases and $G_\uparrow$ at point B decreases. For $t_2=0.7$ and $V_g=-0.32$, the DOS at the Fermi level nearly vanishes while for $V_g=-0.37$ there is a small DOS peak at the Fermi level. Accordingly, in Fig. 5(f) the conductance valley A vanishes and the valley B becomes shallow. In fact, one can also find this feature from the band structure of the polymer. From Figs. 4(a) and 4(c) one can see that for large t_2, due to the flatband, the local DOS just below the middle gap is very large. As t_2 decreases [e.g., $t_2=0.7$ in Figs. 4(b) and 4(d)], the band just below the gap becomes dispersive and the local DOS decreases for the filling $n>\frac{1}{3}$. Therefore, to obtain a large polarization of the conductance there must be a large hybridization t_2 between the carbon atom and the radical.

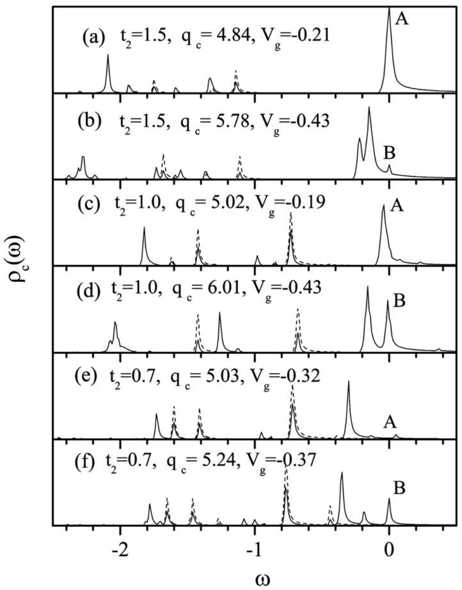

FIG. 6. Local DOS $\rho_c(\omega)$ at cite C of the polymer for $L=6$ and different t_2 and V_g. Other parameters are the same as in Fig. 2. Solid lines and dashed lines correspond to up-spin and down-spin, respectively.

Figure 7 shows the effect of the orbital energy ϵ at radical sites on the conductance. With increasing ϵ, the chemical potential μ_N increases and the valleys move to the left. As ϵ is well below the Fermi level (e.g., $\epsilon=-1.0$), the electrons mainly occupy the radical sites. The DOS at site C is very small so that the valley A in Fig. 7(a) nearly disappears. As ϵ increases, the depth of the valley A increases. For large enough ϵ the conductance is almost fully polarized. Although for small ϵ (e.g., -0.5), the polarization has considerable size at valley B, the fully polarized conductance cannot be realized. Therefore, to design a spin filter one should choose a radical with large orbital energy. For an isolated polymer *poly*-BPO, the Anderson-like model ($U_2=0$) has shown that the transition from a ferromagnetic state (FM) to an antiferromagnetic (AFM) state is present at a critical ϵ.[21] In fact, if U_2 is turned on this transition also exists. The calculation shows that for $t_2=1$, $U_2=3$ and at the half-filling $q_c=6$, the total spin of the polymer changes from $S=1$ to $S=0$ as ϵ increases to a critical value $\epsilon_c=1.15$. Figure 7(f) shows the conductance for $\epsilon=1.2$. The polarization at the valley B disappears while the valley A still exhibits large spin polarization. This indicates that the device can be used to detect the FM to AFM transition in the polymer. Moreover, no matter whether the transition occurs the spin filtering effect can be realized.

The on-site Hubbard repulsion U_2 at radical affects the Coulomb oscillation by changing the chemical potential μ_N of the polymer. The calculation shows that as U_2 is enhanced μ_N increases and the valleys of conductance move to the left. However, the valley A still has perfect polarization. The basic physics does not depend on a specific U_2.

In summary, we have proposed a spin filter based on an organic polymer coupled to a quantum wire. The spin polarization of the conductance is controlled by the gate voltage but not by the external magnetic field. Our results show that a class of organic polymer with flatband ferromagnetism can be candidates of the device. To generate fully polarized conductance, the radical of the polymer must have large orbital energy and hybridization with the carbon atom. As an application of the result, the device can be used to detect the magnetic transition of the polymer.

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