Spin filtering by ferromagnetic nanowires

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We show that electrical current flowing through nanowires made of ferromagnetic disordered alloys can become highly spin polarized.

The increasing ability to control spin-dependent phenomena in condensed matter physics is opening exciting possibilities for the electronic industry. The search for efficient spin filtering systems in particular is very important for spin-based electronics and quantum computation. Spin polarized electrical current for example may be required to operate qubits in some proposed device schemes for quantum computations.

Recently, a clever and promising technique has been devised for fabricating very thin metallic nanowires, with diameters smaller than 10nm. It uses suspended carbon nanotubes as substrates for deposition by electron-beam evaporation of several metals, including Fe and Ni. By initially coating the carbon nanotube with a small amount of Ti (with nominal thicknesses ranging from 1-2nm) other metals can stick more easily to the substrate, leading to the formation of nice continuous nanowires up to tens of microns long.

The purpose of this letter is to show that electrical current flowing through nanowires of ferromagnetic disordered alloys can become highly spin polarized. Therefore, wires with such characteristics may be useful as spin injectors in electronic devices. We begin by presenting and discussing the main physical mechanisms that are responsible for the spin filtering behavior of these systems. Then we perform model calculations to illustrate how effective those mechanisms can be, and finally discuss our results and the guidelines they provide for choosing the nanowire composition that may maximize the spin filtering effect.

It is well known that disorder in metallic systems may lead to localization. Depending on the nature and degree of disorder, localized states may appear near the top and bottom of the conduction bands of three dimensional metallic systems, with a mobility edge separating localized from extended states. Non-interacting disordered electronic systems with lower dimensionality in the thermodynamic limit have localized states only. Strictly speaking they are insulators at zero temperature. In fact, localization effects can be very effective in reducing the conductance of nanowires. They can make the average conductance fall off exponentially with the wire length \( \ell \) for sufficiently long wires. The localization length \( \Lambda \) is determined by the asymptotic decaying rate of \( g \), being shorter the faster \( g \) decreases. Nikolić and MacKinnon have made a detailed study of the electrical conductance in non-magnetic disordered nanowires, employing a single-band tight-binding model to describe the electronic states. The problem involves basically four characteristic lengths: \( \ell, \Lambda \), the wire width \( w \), and the electronic mean free path \( \lambda \). In their work, they illustrated the occurrence of different transport regimes according to existing relations between \( \ell, \lambda, \) and \( \Lambda \). Transport is quasi ballistic, when \( \ell \) is comparable with \( \lambda \), mesoscopic when \( \lambda < \ell < \Lambda \), and strongly localized when \( \Lambda < \ell \). The quantities \( \lambda, \Lambda \), and \( g \) are all functions of energy, and the conductance may change regime as the energy varies. Actually, in the presence of bulk disorder they found that \( g \) decays faster as a function of \( \ell \) for energies close to the band edges in the strong localization regime.

It is noteworthy that the scattering of carriers in metallic ferromagnets is generally spin dependent, even when the scattering potentials do not depend upon spin. This is mainly due to the densities of states around the Fermi energy being different for majority and minority spin carriers. In ferromagnetic transition metals, for example, the spin polarization of the sp-electrons is relatively small compared with that of the d-electrons. Both sp and d-electrons participate in electrical conductance, but the d-electrons are less mobile because they have a larger effective mass. Nevertheless, even assuming the current is predominantly carried by sp-electrons in such systems, sp-d hybridization may lead to distinct conductances for up and down spins. The reason, as rightfully argued by Mott, is that electrical resistance is proportional not only to the density of scattering centers, but also to the number of available states where electrons can scatter into. Thus, the existence of unoccupied d states at the Fermi energy \( E_F \) in transition metals acts as a trap for the sp electrons, because sp-d hybridization allows them to be scattered into the available d-states. Since the densities of available d-states at \( E_F \) differ for up and down spins in ferromagnetic transition metals, it follows that the electronic mean free paths of majority and minority spin carriers are usually not equal in such systems. Furthermore, the atomic potential fluctuations experienced by d electrons in transition metal alloys are often much
larger than those felt by s electrons. As a consequence, s and d electrons are differently affected by disorder, and we will show that the localization lengths for majority and minority spin electrons may be also rather different in ferromagnetic nanowires made of transition metal alloys. In such systems $\lambda_1$ and $\Lambda_1$ are both energy and spin dependent quantities.

An additional relevant length scale for discussing spin dependent transport in ferromagnets is the mean free path associated with spin flip scattering ($\lambda_f$). In metallic systems $\lambda_f$ is usually much longer than $\lambda$. For nanowires with $\ell < \lambda_f$, the conductances for up and down spins are independent, hence $\tilde{g} = \tilde{g}_f + \tilde{g}_l$, where $\tilde{g}_f$ is the average conductance for electrons with spin $\sigma$. The up- and down-spin channels in this case behave as resistors in parallel. Since both $\tilde{g}_f$ and $\tilde{g}_l$ depend upon energy, they may decay as functions of $\ell$ with different rates, particularly in strong ferromagnets where the majority d-bands are completely filled. With dissimilar localization lengths for up and down spin carriers, the polarization of the electrical current may thus increase very rapidly with $\ell$.

To illustrate how effective these mechanisms can be, we perform model calculations for ferromagnetic nanowires made of metallic disordered alloys. For numerical simplicity we consider two-dimensional wires of finite length, sandwiched by perfect leads. Experimentally the wire thickness is not constant, and this is simulated by assuming it fluctuates randomly by $\pm \delta w$ around an average width $\bar{w}$. In order to allow spin dependent Mott scattering mechanism to take place, the nanowire electronic structure is described by a simple s-d model Hamiltonian

$$H = \sum_{ij\sigma} \sum_{\mu \nu} h_{ij}^{\mu\nu} a_{i\mu\sigma}^\dagger a_{j\nu\sigma} + \sum_{i\mu} U_i^{\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} ,$$  

where $a_{i\mu\sigma}^\dagger$ is the creation operator for an electron with spin $\sigma$ in orbital $\mu$ on site $i$, and $n_{i\mu\sigma}$ is the corresponding occupation number. The sp- and d-orbital sets in transition metals are represented here by just two s orbitals labeled by $\mu = 1, 2$, respectively. The on-site matrix elements $h_{ij}^{\mu\nu} = e_i^{\mu} \delta_{\mu\nu} + (1 - \delta_{\mu\nu}) \gamma_i$, where $e_i^{\mu}$ are atomic energies, and $\gamma_i$ characterizes the hybridization between the s and d bands. Our system consists of a ferromagnetic disordered alloy, where sites are occupied with a certain probability either by magnetic or non-magnetic metal atoms. We neglect the effect of disorder in the hopping integrals, and consider them as being non zero between nearest neighbor sites only. Thus, for nearest neighbor sites $i \neq j$, $h_{ij}^{\mu\nu} = -t^{\mu\nu} \delta_{\mu\nu}$, where $t^{ss}$ and $t^{dd}$ symbolize the transfer integrals for s and d electrons, respectively. $U_i^{\mu}$ represents the Coulomb interaction between electrons located on the same site and orbital, and we further assume it takes place only when they occupy the d-orbitals of the magnetic metal atoms.

In principle all the parameters involved here can be estimated from the band structures or renormalized atomic potentials of the constituent metals. However, given the model nature of our calculation we have selected representative values for the parameters, rather than attempting to adjust them to fit a specific system. For example, we choose our energy unit such that $t^{ss} = 1$, and take $t^{dd} = 0.2$, and $\gamma_i = 0.9$ independent of the lattice sites. This approximately reproduces the typical bandwidths of transition metals. By placing the band structures of the constituents on the same absolute scale, and aligning the corresponding Fermi energies, one may also estimate the energy levels $E_i^{s,d}$, characterizing the host ($H$) and impurity ($I$) metals. We shall discuss alloys based on ferromagnetic transition metal alloys such as Fe, Co or Ni, with non-magnetic transition metal impurities of the left side of those elements in the periodic table. We thus set $E_i^H = 0$ as our energy origin, and choose $E_i^I = 0$, $E_i^I = 0.03$, and $E_i^I = 0.6$ or 0.9, as a reasonable set of values for describing representative systems in the scope of such simple a model.

We treat the electron interaction within the Hartree-Fock approximation, thus reducing the on-site interaction term to $-\frac{1}{2} \sum_{ij} \delta_{\mu\sigma} \delta \sigma$, where $\Delta_i^{\mu\sigma}$ represent the exchange splittings for the s and d orbitals, and $\sigma = \pm 1$ for $\uparrow$ and $\downarrow$ spins, respectively. With the simple form of interaction assumed, only $\Delta_i^{\uparrow\downarrow} \neq 0$, corresponding to a molecular field acting solely on the d orbitals of the magnetic-metal host atoms.

Since our wire may be viewed as a sequence of atomic chains of finite sizes $\bar{w} \pm \delta w$, it is convenient to label the atomic site positions by a pair of indices $(l, r_l)$ representing the line $l$ the atom belongs to, and its position $r_l$ along that line. The conductance in the spin channel $\sigma$ is calculated by the Kubo formula

$$g_\sigma(E) = \frac{4e^2}{h} \text{ReTr} \overline{G_{00}^{\sigma\sigma} G_{11}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} - t_{01} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma} G_{10}^{\sigma\sigma} G_{01}^{\sigma\sigma}$

where 0 and 1 symbolize any two adjacent line indices (the choice is arbitrary due to current conservation), and $t_{01}$ is the tight-binding hopping matrix between such lines. $G_{lm}^{\sigma\sigma}$ are matrices representing the advanced and retarded one-electron propagators for particles with spin $\sigma$, evaluated at energy $E$, connecting lines $l$ and $m$. ReTr stands for the real part of the trace over all orbitals and line sites, and $e^2/h$ is the quantum conductance.

The required one-electron Green functions were calculated by the method described in reference [8]. Firstly, the surface Green functions of the semi-infinite perfect leads are generated by a well established technique. Then, the Dyson equation is employed recursively to built the corrugated disordered wire parts atop the leads to the left and right of lines 0 and 1, respectively. Finally, those wire parts are reconnected by turning on the electron hopping $t_{01}$ between them. In our calculations the impurity sites are randomly chosen for a given alloy concen-
tration, and configurational averages of \( g_\sigma \) are performed over 4,000 different samples.

Before presenting our results for ferromagnetic systems, it is instructive to study the conductance of non-magnetic disordered wires with this simple s-d model, particularly the behavior of \( \bar{g} \) as a function of \( \ell \) for different values of energy. Thus, we start by setting \( \Delta_H^d = 0 \), and consider wires with \( \bar{w} = 10 \) atoms, \( \delta \bar{w} = \pm 1 \) atom, sandwiched by leads of width \( w_L = \bar{w} \) (leads of larger widths play no significant role on the main points we wish to address). Figure 1 shows localization lengths calculated as functions of energy for different impurity potentials and concentrations. Here, it is statistically more appropriate to define \( \tilde{g} = \exp[\ln \bar{g}] \), where \( (f) \) denotes the configurational average of \( f \). \( \Lambda \) is determined by fitting the asymptotic exponential decaying rate of \( \tilde{g} \) with \( \ell \); more precisely, \( \Lambda^{-1} = -\partial \tilde{g} / \partial \ell \) for \( \ell \gg 1 \). The localization length clearly depends upon the impurity potential strength relative to the host, i.e., on \( \Delta_x^d = \epsilon_f - \epsilon_H^d \). It is also evident that \( \Lambda^{-1} \) increases as energy approaches the d-bands region (delimited here by \( \approx \epsilon_\ell \pm 0.8 \) for non-hybridized bands), where conduction electrons have more states to be scattered into. States in this energy range are more affected by impurity concentration changes because \( | \Delta_x^d | \gg | \Delta_x^s | \). The most striking feature, however, is the very pronounced maximum that appears in \( \Lambda^{-1} \) near the top of the d band, for reasonably large positive values of \( \Delta_x^d \). The maximum becomes bigger and broader with increasing impurity concentration, and corresponds to a considerably faster decaying of \( \tilde{g} \) with \( \ell \), as illustrated in the inset of figure 1(a). It arises from an interesting combination of disorder, hybridization and screening effects in the nanowire. To understand its physical nature we recall that hybridization mixes the s- and d-conducting channels, and d-states are more directly affected by disorder in transition metal alloys. Screening in such systems is also very effective, and can cause significant changes in the local density of states (LDOS) around the impurity sites. It is well known that resonances and virtual bound states may appear near \( E_F \), depending on the relative strength of the impurity potential. At sufficiently low temperatures, the conduction electrons are scattered predominantly into available states near the scattering centers. Therefore, impurity resonant states at \( E_F \) may strongly influence electrical conductance, especially in disordered metallic systems. We notice that the energy position and some features of the \( \Lambda^{-1} \) maximum are closely related to the impurity potential strength. This is illustrated in the inset of figure 1(b), where we compare the LDOS on a single impurity site, and its averaged value over the impurity neighboring sites, with \( \Lambda^{-1} \); all calculated in the same energy range for \( \Delta_x^d = 0.6 \), but smaller values of \( x = 0.05 \), and \( \gamma = 0.2 \), in order to highlight the virtual bound state structure in the LDOS. The peaks in \( \Lambda^{-1} \) and in the LDOS are clearly correlated in this case, as expected.

In fact, screening and disorder effects in ferromagnetic transition metal alloys can be highly spin dependent. In some Ni based alloys, screening is done largely by down-spin electrons, whereas up-spins normally play a significant part in Fe based alloys. Ni\(_{1-x}\)Ti\(_x\), for instance, is a classical example where the introduction of a Ti impurity leads to an up-spin bound state being pushed completely above \( E_F \). The characters of up- and down-spin conducting states can certainly be altered by varying the alloy constituents and composition. To illustrate how appropriate combinations of elements may lead to very large spin filtering effects, we finally consider a ferromagnetic disordered nanowire attached to two non-magnetic metallic leads. We assume a typical value of exchange splitting \( \Delta_H^d = 0.5 \) on the d orbitals of the magnetic host atoms, and choose \( E_F = 1.2 \), corresponding to a strong

![Figure 1: Inverse localization lengths calculated for a non-magnetic disordered wire as functions of energy for different impurities (\( \Delta_x^d = 0.9 \) (a); \( \Delta_x^d = 0.6 \) (b)), and concentrations \( (x = 0.1 \) (dashed line); \( x = 0.2 \) (solid line)). The inset in (a) shows the average conductance (calculated for \( \Delta_x^d = 0.9 \) and \( x = 0.2 \) plotted against the wire length \( \ell \) for distinct values of energy: \( E_F = 2.4 \) (dashed line), \( E_F = 1.2 \) (dot-dashed line), and \( E_F = 0.8 \) (solid line). Lengths and energies are measured in units of the lattice spacing and s-hopping integral, respectively. The inset in (b) shows the LDOS (in arbitrary units) on an impurity site (dashed line), and averaged over its surrounding sites (thin solid line), together with \( \Lambda^{-1} \) (thick solid line), all calculated in the same energy range for \( \Delta_x^d = 0.6 \), but smaller values of \( x = 0.05 \), and \( \gamma = 0.2 \).]
inset of figure 2, where rapidly with the wire length. This is represented in the contrasting with the much less mobile and predominant down-spins. Such a remarkable behavior is basically due to the large s character of the up-spin conduction states, calculated as functions of the lattice spacing and s-hopping integral, respectively. The inset shows the percentage fraction of up-spin conductance $P = \bar{g}_\uparrow / \bar{g}$ plotted against $\ell$ for $E_F = 1.2$ (solid line) and $E_F = 0.35$ (dot-dashed line), corresponding to a strong and weak ferromagnet, respectively.

ferromagnet with its up-spin d band completely filled. Our results for $\bar{g}_\uparrow$ and $\bar{g}_\downarrow$, calculated as functions of $\ell$, are shown in figure 2. They depict $\bar{g}_\downarrow$ decreasing much faster than $\bar{g}_\uparrow$, showing that the localization length of up-spin electrons in this case is much larger than that of the down-spins. Such a remarkable behavior is basically due to the large s character of the up-spin conduction states, contrasting with the much less mobile and predominant d character of the down-spin ones. As a consequence, the percentage fraction of up-spin conductance increases rapidly with the wire length. This is represented in the inset of figure 2, where $P = \bar{g}_\uparrow / \bar{g}$ is plotted against $\ell$ for two different values of $E_F$, corresponding to a strong and weak ferromagnet, respectively. One immediately sees that very high spin polarized electrical currents can be achieved with relatively short ferromagnetic disordered nanowires, just a few hundred atoms long. This makes them excellent candidates for being used as spin injectors in nanoelectronic devices.

In summary we have shown that localization lengths of up- and down-spin electrons may be rather different in ferromagnetic disordered nanowires. As a result, electrical currents flowing through such structures may acquire a high degree of spin polarization. The localization lengths for up and down spins are determined mainly by the character of the electronic states around the Fermi energy. By judiciously choosing the nanowire alloy constituents and concentration, one can certainly modify such characters, and perhaps even control those localization lengths. There is a large ground for experimenting with such systems. Presently, the nanowires reported in reference[4] are composites of a carbon nanotube in the core, covered by a relatively small amount of Ti, and a second metal on the outside. Nevertheless, careful heat treatments, and simultaneous deposition of different metals, may possibly be employed to fabricate nanowires of ferromagnetic disordered alloys. The most obvious choices to start with would be NiTi and FeTi alloys. The Ti impurity potential strength is relatively stronger in Ni alloys, but the magnetization of FeTi remains finite for larger concentrations of Ti. Other transition metal combinations, may deserve to be examined. The fact that both Ni and Fe separately form continuous nanowires, suggests that NiFe alloys with virtually any concentration may also do, thus broadening the possibilities for exploring different spin dependent characteristics of the conducting states. NiCr alloys, with the Fermi level sitting on an up-spin virtual bound state, seems an interesting system too. The spin filtering mechanism reported here relies on localization and hybridization effects. Most importantly, on the existence of relatively large contrast between the conduction state characters of up and down spins in the nanowires. We hope our findings will stimulate further investigation on these systems.

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