Spin Torques in Ferromagnetic/Normal Metal Structures

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Recent theories of spin-current-induced magnetization reversal are formulated in terms of a spin-mixing conductance $G^{\text{mix}}$. We evaluate $G^{\text{mix}}$ from first-principles for a number of (dis)ordered interfaces between magnetic and non-magnetic materials. In multi-terminal devices, the magnetization direction of a one side of a tunnel junction or a ferromagnetic insulator can ideally be switched with negligible charge current dissipation.

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“Giant magnetoresistance” refers to the large change of resistance brought about by applying an external magnetic field so as to change the angle between the magnetization directions of adjacent magnetic films \cite{10}. Since a spin injected into a magnetic material experiences a torque, it has been argued that there should be a reverse effect, namely, that passage of a current through adjacent magnetic layers should lead to the transfer of spin angular momentum from one layer to the other \cite{10} with possible reorientation of the magnetizations for sufficiently large currents \cite{10}. Interestingly, the sign of the corresponding torque should be reversed on changing the current direction leading to the possibility of making an electronically accessible non-volatile magnetic memory whose performance on downscaling would appear to compare favorably with other alternatives \cite{10}. The experimental observation of current-induced magnetization reversal (“spin transfer”) effects by a number of groups \cite{10} calls for a more general framework for electrical transport in non-collinear and disordered magnetic systems. Two suitable and nearly equivalent approaches are the circuit theory based on kinetic equations for spin currents \cite{10} and the random matrix theory of transport in magnetic heterostructures \cite{10}.

In the circuit theory, the torque and current are formulated in terms of (real) spin-up and spin-down conductances $G^\uparrow$ and $G^\downarrow$ and a new spin-mixing conductance $G^{\text{mix}}$ which is complex. The mixing conductance has only been studied using simple free electron models and little is known about its dependence on real material parameters. Since free-electron models miss an important contribution to spin transport in layered magnetic materials coming from the mismatch of the complex $d$ bands responsible for itinerant ferromagnetism \cite{10}, it is important to take this into account when evaluating $G^{\text{mix}}$ for realistic interfaces.

In this paper we use methods recently developed \cite{10} to calculate the scattering matrix within the framework of density functional theory in order to evaluate the spin- and spin-mixing conductances for a number of systems of current interest. We show that the spin-mixing conductance in tunnel junctions can remain large even when the conventional conductance itself is made vanishingly small, which has not been anticipated previously and should be important in utilizing the spin-torque effects. We suggest a configuration in which this effect could be observed.

We begin with two basic elements of a magnetic circuit: a non-magnetic (NM) element in which there is a spin-accumulation in the direction $\mathbf{s}$ [as a result of injection from elements of the circuit e.g. by a source-drain current in Fig. 1(a)] and a ferromagnetic (FM) element whose magnetization is given by the unit vector $\mathbf{m}$. In general $\mathbf{s}$ and $\mathbf{m}$ are non-collinear and it is convenient to split the $2 \times 2$ matrix current $\mathbf{f}$ from the non-magnetic element into the ferromagnetic element into a scalar charge current $I_0$ and a vector spin current $\mathbf{I}_s$: $\mathbf{f} = (I_0 + \sigma \cdot \mathbf{I}_s)/2$ where $\sigma$ is a vector of Pauli spin matrices,

$$
\mathbf{I}_s = \mathbf{m}[(G^\uparrow - G^\downarrow)(f^\uparrow_p - f^\downarrow_N) + (G^\uparrow + G^\downarrow)\Delta f^\uparrow]
+ (G^\uparrow + G^\downarrow - 2\text{Re}G^{\text{mix}})(\mathbf{s} \cdot \mathbf{m})\Delta f^N
- 2\text{Re}G^{\text{mix}}\Delta f^N + 2(\mathbf{s} \times \mathbf{m})\text{Im}G^{\text{mix}}\Delta f^N,
$$

(1)

and $\hat{f}^N = f^N + \sigma \cdot \mathbf{s} \Delta f^N$ and $\hat{f}^F = f^F + \sigma \cdot \mathbf{m} \Delta f^F$ describe the deviation of the distribution functions in the NM and FM nodes, respectively, from their equilibrium values \cite{17}. When a spin-current is injected into a ferromagnetic material, the component of $\mathbf{I}_s$ perpendicular to the magnetization direction $\mathbf{m}$ (times the Bohr magneton and gyromagnetic ratio) equals the torque act-
ing on the ferromagnet [11] and this is seen to be determined entirely by the real and imaginary parts of \( G^{\text{mix}} \). The spin-up, spin-down and spin-mixing conductances characterizing transport through an interface are defined as \( G^\uparrow = \frac{e^2}{h} \text{tr}(t^\uparrow_1 t^\downarrow_1) \), \( G^\downarrow = \frac{e^2}{h} \text{tr}(t^\downarrow_1 t^\uparrow_1) \) and \( G^{\text{mix}} = \frac{e^2}{h} \text{tr}(I - r^\uparrow_1 r^\downarrow_1) \), in terms of the spin-dependent transmission and reflection matrices \( t(\upsilon) \) and \( r(\upsilon) \): \( I \) is an \( M \times M \) unit matrix where \( M \) is the number of conducting channels in the NM element [11,13]. Note that the mixing conductance can be measured in principle by the angular magnetoresistance of perpendicular spin valves [13] analyzed by circuit theory [19].

The parameter-free calculation of the transmission and reflection matrices [16] is based on the surface Green’s function method [20] implemented with a tight-binding linear muffin tin orbital basis [21]. The calculation time scales linearly with the number of layers in the scattering region and as the cube of the size of the in-plane unit cell. Because a minimal basis set is used, we are able to perform calculations for lateral supercells containing as many as 10 \( \times \) 10 atoms and to model disorder very flexibly within such supercells without using any adjustable parameters. The electronic structure is determined self-consistently within the local spin density approximation. For disordered layers the potentials are determined self-consistently using the layer CPA approximation [20]. The calculations are carried out with a \( k_\parallel \) mesh density equivalent to more than 3600 mesh points in the two-dimensional Brillouin zone (BZ) of a 1 \( \times \) 1 interface unit cell. The results of calculations for clean and disordered fcc(111) Cu/Co and bcc(001) Cr/Fe metallic interfaces and for an fcc(111) Cu/Co/Vac/Co tunneling configuration are given in Table 1.

We first discuss our results for the Cu/Co and Cr/Fe interfaces. Both have been the subject of much study in the context of exchange coupling and giant magnetoresistance and different calculations of the interface transmission matrices yield very similar results for the spin-dependent interface resistances [7,10]. The atomic volume of each pair of materials is very similar and we model disordered interfaces using a 2 layer thick 50-50 alloy of the component materials. The results given in the Table do not depend sensitively on the alloy concentration used.

For a clean Cu/Co(111) interface, the real part of the mixing conductance is comparable in size to the spin-up and spin-down conductances but the imaginary part is almost a factor of 50 smaller. Interface disorder increases the mixing conductance, the real part by about 35%, the imaginary part by a factor of three.

It is interesting to compare \(|G^{\text{mix}}|\) with \( G^\uparrow + G^\downarrow \). The mixing conductance mainly contributes to the torque while \( G^\uparrow + G^\downarrow \) determines the electron current. Large values of \(|G^{\text{mix}}|/(G^\uparrow + G^\downarrow)\) mean more torque per unit current. The calculations show that disorder at the Co/Cu interface increases the spin-torque. Another possibility to increase the ratio of \(|G^{\text{mix}}|\) to \( G^\uparrow + G^\downarrow \) is to insert an impurity layer on the Cu side; a Co monolayer inserted on the Cu side scarcely changes the mixing conductance but reduces the normal conductance significantly.

For the Cr/Fe interface the band structure matching and the effect of interface disorder are quite different compared to Cu/Co. Whereas the majority spin states of Co/Cu match very well, it is the minority spin-states in Cr and Fe which match best; see Figs. 1(c,d). For a perfect Cr/Fe(001) interface, the mixing conductance is almost twice as large as the normal conductance. The expression for the mixing conductance shows that having a large number of propagating channels on the non-ferromagnetic side of the interface can lead to a large mixing conductance.

It is of interest to have a closer look at the \( k_\parallel \) resolved mixing conductance \( G^{\text{mix}} \). We can see from Fig. 1(e) that close to the center of the Brillouin zone (BZ) the real part of the \( G^{\text{mix}} \) is very large, even larger than the number of channels in Cr at the same \( k_\parallel \)-points, shown in Fig. 1(b); at the same \( k_\parallel \)-points the transmission of majority spin electrons is very low. Thus at some \( k_\parallel \) the mixing conductance can be much larger than the normal conductance. This can be understood in terms of a simple one-dimensional infinite barrier model in which the spin-up and spin-down barriers are displaced in space by an amount \( \Delta \). For both spins the reflection amplitude is 1. However, the displacement \( \Delta \) introduces a phase shift \( e^{-2ik_\parallel \Delta} \) for electrons with wave-number \( k \) so that the mixing conductance can have any value \( G_0(1-e^{-2ik_\parallel \Delta}) \) for this simple single-channel model. Although \( G^{\text{mix}} \) is large around \( k_\parallel = 0 \) for Fe/Cr, the minority-spin reflection is very low in most parts of the BZ so that after averaging over the BZ, \( G^{\text{mix}} \) is not very high compared with the normal conductance.

The imaginary part of \( G^{\text{mix}} \) is related to the spin precession which results from the non-collinear alignment of the spins of the injected electrons and the magnetization (or an external magnetic field). A non-vanishing imaginary part of the mixing conductance, \( \text{Im} G^{\text{mix}} \), should result in asymmetry with respect to time reversal [22,23]. However, \( \text{Im} G^{\text{mix}} \) is small in all the systems we have studied. The reason for this can be understood by examining the \( k_\parallel \) resolved imaginary part of \( G^{\text{mix}} \) shown in Fig. 1(f). \( \text{Im} G^{\text{mix}} \) can be negative as well as positive and it is the partial cancellation of these contributions which leads to the net result being small. This can be illustrated using the simple phase-shift model as follows. Suppose that the phase shift of the reflected waves \( \delta(k_\parallel) \) is distributed randomly between \( \varphi_1 \) and \( \varphi_2 \) with equal weights and that the amplitude of \( r^\uparrow_1 r^\downarrow_1 \) is \( A \), then the average mixing conductance is

\[
\frac{G_0}{\varphi_2 - \varphi_1} \int_{\varphi_1}^{\varphi_2} (1 - A e^{i \delta}) d\delta = \frac{e^2}{h} \left[ 1 + \frac{iA}{\varphi_2 - \varphi_1} (e^{i\varphi_2} - e^{i\varphi_1}) \right]
\]

where \( G_0 = \frac{e^2}{h} \). If \( \varphi_1 = -\varphi_2 \) then \( \text{Im} G^{\text{mix}} \) is zero and
Re $G^{mix} = G_0$. In a more realistic treatment the weights will not be homogeneous and $\varphi_1$ will be slightly different from $-\varphi_2$ so that Im $G^{mix}$ is not exactly zero. To obtain a large Im $G^{mix}$ experimentally, one should use a material with a small number of conducting channels such as a semiconductor as the non-magnetic element. Also in a ferromagnetic insulator Im $G^{mix}$ could be significant [23].

We may conclude that a large reflection amplitude does not mean that the mixing conductance must be small. It provides us with a means to realize large values of $|G^{mix}|/(G^\uparrow + G^\downarrow)$ by using a tunnel junction or ferromagnetic insulator as the FM element. For such non-conducting interfaces we predict that it will be possible to obtain a non-zero spin current while the electronic current is zero or vanishingly small. We confirm this by calculating the mixing conductance for a Cu/Co/Vac/Cu tunnel junction, here we use 6 layers empty spheres to model the barrier. The mixing conductance is found to be 0.41 – 10.04 and 0.53 – 10.003 for clean and dirty systems, respectively, in units of $10^{15} \Omega^{-1} m^{-2}$, which very close to the mixing conductances of Cu/Co interfaces. The normal conductance is of the order of $10^{-11}$ in the same system. For even thicker layers the torque simply equals that of the metallic interface and the tunnel junction only suppresses the charge current.

To inject a spin-current in the absence of an electron current we need to consider a three terminal device (“spin-flip transistor”) such as that sketched in Fig. 1(a) [24]. A current from FM1 into FM2 induces a spin-accumulation in the NM node which is easily calculated [24]. Here we simply assume that a spin-accumulation exists in NM and analyze what happens when FM is a magnetic insulator or is the top magnetic element of a magnetic tunnel junction. In the latter case it is possible to independently determine the orientation of FM by means of the tunneling magnetoresistance [24]. The spin torque is that of the metallic junction, but without the energy dissipation caused by the particle current. In practical memory devices it may be advantageous to be able to achieve this separation of particle and spin injection.

In summary, we have studied the mixing conductance of Cu/Co, Cr/Fe and Cu/Co/Vacuum/Co configurations taking the full transition metal electronic structure into account and including disorder. The effect of the mixing and normal conductances can be separated for a three terminal device where one of the terminals is a ferromagnetic insulator or a magnetic tunnel junction for which the normal conductance can be made vanishingly small without affecting the size of the mixing conductance.

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FIG. 1. (a) Sketch of a three-terminal device where a normal metal (NM) element is connected to three ferromagnetic elements FM1, FM2 and FM. An applied bias causes a current to flow between FM1 and FM2. If FM is a tunnel junction or a magnetic insulator then the particle flow into FM should be vanishingly small. (b) Number of propagating channels in first Brillouin Zone for bulk Cr. For a clean Cr/Fe interface (c) and (d) show the minority-spin and majority-spin conductances, (e) and (f) the real and imaginary parts of the mixing conductance. Units of conductance are \( e^2/h \). The result of integrating over the whole Brillouin Zone is given in brackets at the top of each panel. Note that the values represented by color differ per panel but with the zeros are represented by the green color.

| system                        | interface   | \( G^{\text{maj}} \) | \( G^{\text{min}} \) | Re\( G^{\text{mix}} \) | Im\( G^{\text{mix}} \) |
|-------------------------------|-------------|-----------------------|-----------------------|------------------------|------------------------|
| Cu/Co(111)                    | Clean       | 0.42                  | 0.36                  | 0.41                   | 9.2 \times 10^{-3}     |
| Cu/Co(111)                    | 2\times 50-50 alloy | 0.42                  | 0.33                  | 0.55                   | 3.0 \times 10^{-2}     |
| Cu/Co(1)/Cu(7)/Co(111)        | Clean       | 0.40                  | 0.22                  | 0.41                   | 3.2 \times 10^{-2}     |
| Cu/Co(1)/Cu(7)/Co(111)        | 2\times 50-50 alloy | 0.41                  | 0.21                  | 0.55                   | 3.6 \times 10^{-2}     |
| Cr/Fe(001)                    | clean       | 0.14                  | 0.35                  | 0.61                   | 2.8 \times 10^{-2}     |
| Cr/Fe(001)                    | 2\times 50-50 alloy | 0.26                  | 0.34                  | 0.61                   | 5.2 \times 10^{-1}     |
| Cu/Co/Vac/Co                  | clean       | 9.3 \times 10^{-12}   | 1.9 \times 10^{-11}   | 0.41                   | -4.1 \times 10^{-2}    |
| Cu/Co/Vac/Cu                  | 2\times 50-50 alloy | 3.3 \times 10^{-11}   | 3.0 \times 10^{-11}   | 0.53                   | 3.3 \times 10^{-3}     |

TABLE I. Interface conductances in units of \( 10^{15} \Omega^{-1} \text{m}^{-2} \).
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