Boltzmann Test of Slonczewski’s Theory of Spin Transfer Torque

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We use a matrix Boltzmann equation formalism to test the accuracy of Slonczewski’s theory of spin-transfer torque in thin-film heterostructures where a non-magnetic spacer layer separates two non-collinear ferromagnetic layers connected to non-magnetic leads. When applicable, the model predictions for the torque as a function of the angle between the two ferromagnets agree extremely well with the torques computed from a Boltzmann equation calculation. We focus on asymmetric structures (where the two ferromagnets and two leads are not identical) where the agreement pertains to a new analytic formula for the torque derived by us using Slonczewski’s theory. In almost all cases, we can predict the correct value of the model parameters directly from the geometric and transport properties of the multilayer. For some asymmetric geometries, we predict a new mode of stable precession that does not occur for the symmetric case studied by Slonczewski.

In 1996, Slonczewski and Berger predicted that an electric current flowing through a magnetic multilayer can exert a spin-transfer torque on the magnetic moments of the heterostructure. This torque can produce stable magnetic precession and/or magnetic reversal, both of which have been widely studied experimentally and theoretically. Figure 1 illustrates a common geometry known as a “spin-valve” where a non-magnetic spacer layer separates a thick “pinned” ferromagnetic layer from a thin “free” ferromagnetic layer. Non-magnetic leads connect the ferromagnets to electron reservoirs.

Slonczewski developed a theory of spin-transfer torque that combines a density matrix description of the spacer layer with a circuit theory description of the remainder of the structure. He worked out the algebra for the case where the spacer layer is thin and the spin valve is symmetric (identical ferromagnets and leads) and found the torque \( L_S \) to be the same on the left and right spacer/ferromagnet interfaces. As a function of the angle between the two ferromagnets,

\[
L_S(\theta) = \frac{\hbar I}{2e} \left( \frac{PA^2}{\Lambda^2 + 1} + (\Lambda^2 - 1)\cos \theta \right).
\]

In this formula, \( I \) is the total current that flows through the structure,

\[
P = \frac{1}{2} \left( R_L - R_R \right) = \frac{r}{R} \quad \text{and} \quad \Lambda^2 = GR.
\]

\( R_L \) and \( R_R \) are effective resistances experienced by spin up and spin down electrons between the reservoir and the spacer layer. The conductance \( G = \frac{e^2 k_F^2}{4\pi^2 \hbar} \), where \( A \) is the cross-sectional area of the device.

In this paper, we solve Slonczewski’s equations for the general asymmetric case and derive formulae for the torques \( L_L(\theta) \) and \( L_R(\theta) \) on the left \((x = x_L)\) and right \((x = x_R)\) spacer/ferromagnet interfaces in Figure 1. We then compare these formulae with numerical results for the torque obtained from a matrix Boltzmann equation.

\[0 = \Delta V_L (1 + \cos^2 \theta) - G^{-1} Q_L \sin^2 \theta - 2 \Delta V_R \cos \theta\]
0 = Q_L(1 + \cos^2 \theta) - G\Delta V_L \sin^2 \theta - 2Q_R \cos \theta. \quad (3)

Two additional equations parameterize the voltage drop differences in terms of effective resistances $R_L$, $R_R$, $r_L$ and $r_R$:

$$\Delta V_L = Q_L R_L + I r_L$$
$$\Delta V_R = -Q_R R_R - I r_R. \quad (4)$$

Finally, Slonczewski derived expressions for the interfacial torques. At $x = x_R$, the torque is

$$L_R = \frac{h}{2e} \frac{Q_R \cos \theta - Q_L}{\sin \theta}. \quad (5)$$

The torque $L_L$ at the $x = x_L$ interface is defined with $Q_R$ and $Q_L$ exchanged.

It is straightforward to solve the four equations (3) and (4) for the four unknowns, $Q_L$, $Q_R$, $\Delta V_L$, and $\Delta V_R$. From these, we find $L_R$ from (5) to be

$$L_R = \frac{h}{2e} \frac{I \sin \theta}{A} \left[ \frac{q_+}{A + B \cos \theta} + \frac{q_-}{A - B \cos \theta} \right] \quad (6)$$

where

$$q_\pm = \frac{1}{2} \left[ P_L \Lambda_L^2 \sqrt{\frac{\Lambda_R^2 + 1}{\Lambda_L^2 + 1}} \pm P_R \Lambda_R^2 \sqrt{\frac{\Lambda_L^2 - 1}{\Lambda_R^2 - 1}} \right]$$
$$A = \sqrt{(\Lambda_L^2 + 1)(\Lambda_R^2 + 1)}$$
$$B = \sqrt{(\Lambda_L^2 - 1)(\Lambda_R^2 - 1)}. \quad (7)$$

The parameters $P_L$, $P_R$, $\Lambda_L$, and $\Lambda_R$ are defined in terms of $R_L$, $R_R$, $r_L$ and $r_R$ as $P$ and $\Lambda$ are defined in (2) in terms of $R$ and $r$. For the symmetric case, $\Lambda_L = \Lambda_R = \Lambda$ and $P_L = P_R = P$. This makes $q_- = 0$ and (6) reduces to Slonczewski’s formula (10) with $L_R = L_L = L_S$. We will see later that the term proportional to $q_-$ in (6) can affect the magnetization dynamics of the spin valve in a qualitative way.

To test (6), we computed the torque on each spacer/ferromagnet interface using a Boltzmann equation formalism. The two ferromagnetic moments in Figure 1 are not collinear, so there is no natural spin quantization axis in the spacer layer. Therefore, we expand the deviation of the semi-classical electron occupation function from its equilibrium value in a basis of Pauli spin matrices:

$$g(k, r) = g_0(k, r) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + g_x(k, r) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$+ g_y(k, r) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + g_z(k, r) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8)$$

In the spacer layer, each of $g_0$, $g_x$, $g_y$, and $g_z$ satisfies a linear Boltzmann equation that takes account of the driving current and of resistive and spin-flip scattering in each material layer. In each ferromagnet and in the adjacent lead, it is sufficient to use $g_0$ and $g_z$ referenced to the fixed direction of magnetization in each. We assume a spherical Fermi surface for each material. We adopt a one-dimensional approximation $g(k, r) = g(k, x)$ and stitch together the solutions in each layer with matching conditions that reflect the complex, spin- and wave-vector-dependent reflection and transmission amplitudes of each interface. The latter are determined from a previously published parameterization.

Electrons that enter a non-magnetic lead from the adjacent reservoir are assumed to have an equilibrium occupation function. For our numerical work, we have chosen material and geometry parameters typical of experiments performed on Cu/Co/Cu/Co/Cu spin valves. The specific numerical values used can be found in Ref. 10. With the final occupation function in hand, it is straightforward to compute the spatially varying voltage, spin accumulation, spin current, and spin-transfer torque. Details will be published elsewhere.

The filled circles in Figure 2 show a typical Boltzmann result for the spin-transfer torque at $x = x_R$ as a function of the angle $\theta$ between the two ferromagnets for an asymmetric geometry. The solid curve in Figure 2 is the same quantity, $L_R(\theta)$, computed from (6). The agreement is excellent, as it is for essentially all other geometries we have studied with thin spacer layers. For comparison, the dashed curve is the Slonczewski torque with the bulk scattering removed. This “interface-only” situation is manifestly symmetric ($q_- = 0$).

For the solid curve plotted in Figure 2, the relative importance of the two terms in (6) is $q_-/q_+ \approx 0.27$. We find that this ratio does not exceed about 0.5 for physically sensible geometries. We will address the qualitative consequences of $q_- \neq 0$ at the end. First, we describe our method to determine the torque parameters $\Lambda_R$, $\Lambda_L$, $P_R$, and $P_L$ that produced the solid curve in Figure 2. We begin by writing an exact expression for the voltage...
\[
\Delta V_L = \int_{-\infty}^{x_L} dx [I_i(x) \rho_i(x) - \hat{I}_i(x) \rho_i(x)]
\]
\[
= \int_{-\infty}^{x_b} dx [\hat{I}_i(x) - \hat{I}_i(x)] \rho(x)
\]  \hspace{1cm} (9)

\( \hat{I}_i(x) \) is \( I_i(x) \) minus the corresponding current in an infinite bulk sample of the material present at point \( x \). The average resistivity in (9) is \( \bar{\rho} = (\rho_1 + \rho_2)/2 \). We will also need the resistivity difference \( \Delta \rho = (\rho_1 - \rho_2)/2 \). Both \( \bar{\rho} \) and \( \Delta \rho \) contain delta functions at the four non-magnet/ferromagnet interfaces to take account of spin-dependent interface scattering.

To make progress, we use a drift-diffusion result\(^{11} \) to the effect that \( I_L(x) \) and \( I_i(x) \) decay exponentially close to the \( x = x_0 \) interface (Figure 1) in both directions. The decay length is the spin-flip length in each material, whether ferromagnet (F) or non-magnet (N). In that case, an approximate expression for (9) is

\[
\Delta V_L = Q_0 \bar{\rho}_N d_{L2}^N + Q_0 \bar{\rho}_F d_{L2}^F + I_0 \Delta \rho F d_{L2}^F + \Delta V_L + \Delta V_C.
\]  \hspace{1cm} (10)

In (10), \( Q_0 = Q(x_0) \). \( \Delta V_L \) and \( \Delta V_C \) are voltage drops at the internal interfaces and at the reservoir contact, and

\[
d_{L2}^F = I_{sf}^F [1 - \exp(-t_{sf}^F/L_{sf})],
\]
\[
d_{L2}^N = I_{sf}^N [1 - \exp(-t_{sf}^N/L_{sf})].
\]  \hspace{1cm} (11)

The effective lengths (11) appear because, due to spin-flip scattering, only electrons within \( d_{L2}^F \) or \( d_{L2}^N \) of the ferromagnetic interfaces can accommodate the dissimilar spin-currents characteristic of the ferromagnets and the non-magnets in equilibrium.

The relationship between \( Q_0 \) and \( Q_L \) is non-trivial\(^{11} \), except when the ferromagnet is very thin (\( t_F^L \ll t_{sf}^L \)). In that case, \( Q_0 \approx Q_L \), and we can connect (10) to (9) and (11) to get

\[
\Lambda^2_L = \frac{G (\bar{\rho}_N \bar{d}_L^N + \bar{\rho}_F t_{sf}^F + R_L + R_C)}{P_L} = \frac{\Lambda^2_{sf} (\Delta \rho F t_{sf}^F + \Delta R_L)}{\Lambda^2_{sf} (\Delta \rho F t_{sf}^F + \Delta R_L)}.
\]  \hspace{1cm} (12)

These two formulae (and similar ones for \( \Lambda_R \) and \( P_R \)), together with (6) and (7) are the principal results of this paper. We used (12) to compute the solid curve in Figure 2. The interface resistance \( G R_L \approx 0.97 \) and contact resistance \( G R_C \approx 1.1 \) were extracted from the Boltzmann solution. \( G R_L \) differs from the experimental value by about 15%\(^{12} \).

The parametrization (6) is well suited to study the behavior of \( L(\theta) \) when we vary the geometry of the magnetic heterostructure and the material parameters in our Boltzmann calculations. For convenience, we did this for symmetric geometries. Figure 3 confirms that \( \Lambda^2 \) is a linear function of \( t_N \) when \( t_{sf}^N \gg t_N \) but saturates when \( t_N \sim t_{sf}^N \). Interestingly, the saturated value of \( \Lambda^2 \) varies linearly with \( t_{sf}^N - t_N \) (\( t_N ^N \) is the inelastic scattering length) rather than with \( t_{sf}^N \) as predicted by (11). For long leads, this can be understood from the fact that conventional resistive scattering is needed to build up non-equilibrium spin accumulation in the non-magnet while spin-flip scattering works to return the non-magnet to equilibrium.

Figure 4 shows the variation of \( \Lambda^2 \) with lead length for different values of the spin-flip length in the ferromagnet. This calculation puts \( t_{sf}^N \rightarrow t_{sf}^* \), so we expect from (11) that \( \Lambda^2 \propto t_N \). This is indeed the case when \( t_{sf}^N \gg t_F^L \). However, when the \( t_{sf}^N \) is comparable (or less than) the ferromagnetic layer thickness, the torque parameter saturates. This is a signal that our approximation \( Q_0 \approx Q_L \) has broken down. In this limit, fast spin-flipping in the ferromagnet reduces \( Q_0 \) to a value much less than \( Q_L \). When that is the case, relatively little spin-flip volume in the non-magnet is needed to reduce the spin current in the non-magnet to zero (its equilibrium value).

A characteristic difference between \( L_2(\theta) \) in (1) for a symmetric geometry and \( L_R(\theta) \) in (3) for an asymmet-
ric geometry can be seen from the difference between the dashed curve and the solid curve in Figure 2. The former has a bump (maximum) in the interval $\pi/2 < \theta < \pi$ only. The latter has a small additional bump in the interval $0 < \theta < \pi/2$ that comes from the $q_- \gamma H$ term. This small change is enough to produce stable magnetization precession for some asymmetric geometries.

Consider a spin valve in the presence of an external magnetic field aligned with the magnetization of the thick ferromagnet. If we ignore shape anisotropy and lattice anisotropy, the total torque acting on the thin ferromagnetic film when electrons flow from right to left in Figure 1 is the sum of the spin-transfer torque $L_H(\theta)$ and a Gilbert damping torque $\gamma H \sin \theta$ (left panel of Figure 5). As the current increases, the spin-transfer torque increases and eventually destabilizes an initial state with parallel moments. Stable precession occurs at angles where the total torque changes from positive to negative (middle panel of Figure 5). When the total torque becomes everywhere positive, the system abruptly switches to the anti-parallel configuration (right panel of Figure 5). There is no regime of stable precession if the zero-current state is anti-parallel.

In summary, we have shown that Slonczewski’s theory of spin-transfer torque in spin-valves can reproduce the results of Boltzmann equation calculations when the non-magnetic spacer layer is thin. When the ferromagnetic layers are also thin, the parameters of the theory can be calculated from first principles. One of us (J.X.) acknowledges support from the National Science Foundation under grant DMR-9820230.

1. J. C. Slonczewski, J. Magn. Magn. Mater. 159, L1 (1996).
2. L. Berger, Phys. Rev. B 54, 9353 (1996).
3. J. A. Katine, F. J. Albert, and R. A. Buhrman, E. B. Myers and D. C. Ralph Phys. Rev. Lett. 84, 3149 (2000); S. Urazhdin, Norman O. Birge, W. P. Pratt, and J. Bass, Phys. Rev. Lett. 91, 146803 (2003); W. H. Ripard, M. R. Pufall, S. Kaka, S. E. Russek, and T. J. Silva, Phys. Rev. Lett. 92, 027201 (2004); A. Fert, V. Cros, J.-M. George, J. Grollier, H. Jaffrès, A. Hamzic, A. Vaurès, G. Faini, J. Ben Youssef, and H. Le Gail, J. Magn. Magn. Mat. 272–276, 1706 (2004).
4. J. Z. Sun, Phys. Rev. B 62, 570 (2000); D. H. Hernando, Yu. V. Nazarov, A. Brataas, and G. E. W. Bauer, Phys. Rev. B62, 5700 (2000); X. Waintal, E. B. Myers, P. W. Brouwer, and D. C. Ralph, Phys. Rev B 62, 12317 (2000); M. D. Stiles and A. Zangwill, Phys. Rev. B 66, 014407 (2002); Z. Li and S. Zhang Phys. Rev. B 68, 024404 (2003); Ya. B. Bazaly, B. A. Jones, and Shou-Cheng Zhang, Phys. Rev. B 69, 094421 (2004).
5. J. C. Slonczewski, J. Magn. Magn. Mater. 247, 324 (2002).
6. M. D. Stiles, A. Zangwill, J. Appl. Phys. 91, 6812 (2002).
7. In the each ferromagnet (and in the adjacent non-magnetic lead), we use the magnetization direction of the ferromagnet to define “up” and “down”. In the non-magnetic spacer, “up” and “down” refer to the spatially-varying direction of local magnetization.
8. The spin current $Q_{\alpha\beta}$ is a second rank tensor. Here, we need only one spatial index (the direction of current flow) and one spin index (the local direction of spin polarization), so a scalar $Q$ is sufficient.
9. M. D. Stiles, D. R. Penn, Phys. Rev. B 61, 3200 (2000).
10. J. Xiao, M. Stiles, and A. Zangwill, to be published.
11. M. D. Stiles, Jiang Xiao, A. Zangwill, Phys. Rev. B 69, 054408 (2004). We have also calculated $L_H(\theta)$ using the drift-diffusion formalism described in this paper. The agreement with Boltzmann is only qualitative.
12. The relationship between the Boltzmann value and the experimental value for the interface resistance is not very straightforward. The experimental values themselves are only accurate to 10% – 20% (Jack Bass, private communication).
13. Slonczewski pointed out in Ref. 3 that the single bump in $L_S(\theta)$ moves from the interval $\pi/2 < \theta < \pi$ to the interval $0 < \theta < \pi/2$ as the coefficient of $\cos \theta$ in $\tilde{\alpha}$ changes sign as a function of $\Lambda$. 