Spin-Transfer Torques: Self-consistent solution of the Spin-Diffusion Equation and the Landau-Lifshitz Equation

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***Abstract*— We present a numerical scheme that allows for the self-consistent treatment of the Landau-Lifshitz equation and the spin-diffusion equation in one space dimension. The scheme is used to simulate magnetic precessions in ferromagnet/normal-metal multilayers that are traversed by strong currents and results are compared to recent experimental observations. The good qualitative and quantitative agreement shows that the diffusive exchange-torque model proposed by Zhang et al. [8] is a legitimate alternative to the ballistic interface-torque model commonly used to describe magnetization dynamics in spin valves.**

I. Introduction

It has been shown that a current injected perpendicular to the planes of a ferromagnet/normal-metal multilayer can lead to dynamical magnetic states in thin soft-magnetic layers [1], [2]. Depending on the magnitude of the currrent, precession or complete reversal of the magnetization is observed. The underlying effect, often called spin-transfer-torque (STT), has been predicted theoretically by Berger [3] and Slonczewski [4] in 1996 and is the topic of ongoing research.

In a macroscopic continuum approach, the dynamics of the direction of magnetization in a ferromagnet (FM) of volume Ω, $\vec{m}(x,t) : \Omega \times \mathbb{R}^+ \to S^2$, is determined by the Landau-Lifshitz equation [5],

$$\partial_t \vec{m} = -\frac{\gamma\mu_0}{1+\alpha^2}\vec{m}\times\vec{H}_{eff} - \frac{\alpha\gamma\mu_0}{1+\alpha^2}\vec{m}\times(\vec{m}\times\vec{H}_{eff}) \quad (1)$$

where γ is the gyromagnetic ratio, μ_0 stands for the magnetic constant, α denotes the damping parameter and $\vec{H}_{eff}$ is the effective field which is proportional to the functional derivative of the free energy of the system with respect to $\vec{m}$. For the description of the STT in a thin magnetic layer of a FM/normal-metal (NM) multilayer structure (called spin-valve), usually one adds to (1) a torque-term of the form

$$\partial_t \vec{m}\Big|_{STT} = c_j \vec{m}\times(\vec{m}\times\vec{m}_F) \quad (2)$$

where c_j is proportional to the current-density traversing the structure perpendicular to the layer planes and $\vec{m}_F \in S^2$ is the magnetization direction of a polarizing thick FM layer. Expression (2) is derived from ballistic transmission/reflection of spin-coherent Fermi-surface-states at a NM/FM interface [4], [6]. The model (2) is well established and has proven to be capable of explaining experimental observations, at least qualitatively [7].

An alternative/complementary approach towards STT has been presented by Zhang et. al [8], who assume that the exchange interaction between conduction electrons and core electrons is responsible for the observed magnetization dynamics. They state that one should treat self-consistently the evolution of the core magnetic moments, determined by (1), and the density of conduction-electron spins, $\vec{s}(x,t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}^3$, determined, for example, by a diffusion equation,

$$\partial_t \vec{s} = D\Delta\vec{s} - \frac{\vec{s}}{\tau} - \frac{J_{ex}}{\hbar}\vec{s}\times\vec{m} \quad (3)$$

where D is the diffusion constant, Δ denotes the Laplacian, τ stands for the spin-flip scattering time and J_{ex} is the exchange constant. Naturally, due to the exchange coupling J_{ex}, the spin density $\vec{s}$ appears in the free energy of $\vec{m}$ and thus in the effective field, which, in the one-dimensional case, we assume to be

$$\vec{H}_{eff} = \vec{H}_{app} + \frac{2K_u}{\mu_0 M_s}(\vec{m}\cdot\vec{u})\vec{u} - M_s(\vec{m}\cdot\vec{w})\vec{w} + \frac{2A_{ex}}{\mu_0 M_s}\Delta\vec{m} + \frac{J_{ex}}{\mu_0 M_s}\vec{s} \quad (4)$$

Here, $\vec{H}_{app}$ denotes the applied magnetic field, K_u the anisotropy constant, M_s the saturation magnetization, A_{ex} the exchange constant, $\vec{u}$ stands for the direction of the magnetic easy axis and $\vec{w}$ is the normal of the easy plane in thin FM layers (the $\vec{w}$-term is missing in thick layers).

Many experimental setups (e.g. in [2]) feature a 5-layer structure like $N_{e1}/F_F/N/F/N_{e2}$, where $N_{e1(2)}$ denote NM-electrodes, F_F is a thick polarising FM layer, N is a NM spacer layer and F is the thin FM layer in which the interesting dynamics take place. To simulate spin-injection into such a system, one can impose a Dirichlet boundary condition $\vec{s}_{inj}$ on equation (3) at the N_{e1}/F_F interface, regardless whether electrons flow from N_{e1} to N_{e2} or vice versa (it is the orientation of $\vec{s}_{inj}$ with respect to $\vec{m}_F$ that changes with the sign of the current). The vector $\vec{s}_{inj}$, by the theory of spin

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injection through an NM/FM junction [9], reads

$$\vec{s}_{inj} = -\vec{m}_F \beta \sqrt{\frac{\tau}{D}} \frac{j}{q} \tag{5}$$

where β is a polarisation parameter which we choose to be 1 throughout this paper, j denotes the current density and q the proton charge. Thus, for $j > 0$ (particle density flow from N_{e1} to N_{e2}), one obtains a vector $\vec{s}_{inj}$ that is antiparallel to $\vec{m}_F$ and vice versa. At the other three interfaces of the five-layer structure one demands continuity of $\vec{s}$ and the spin current, $-D\partial_x \vec{s}$, and at infinity one imposes the homogenous Neumann condition $\partial_x \vec{s}(\infty) = 0$. Equation (3) with the boundary/interface conditions mentioned above has been studied analytically in the case of constant $\vec{m}$ [10], [11]. It is the purpose of this work to go beyond the case of $\vec{m}$=$const.$ in the Zhang-Levy-Fert (ZLF) model [8] and solve the Landau-Lifshitz equation (1) and the spin-diffusion equation (3) self-consistently. The goal is to show that, with reasonable physical parameters, the diffusive ZLF-model is capable of reproducing experimental findings, thereby emphasizing its status as an alternative to the ballistic interface-torque picture, equation (2).

This paper is structured as follows: in section II we present a numerical scheme that solves self-consistently the system (1), (3) in multilayered structures in one space dimension. In section III we apply this scheme to simulate magnetization dynamics in spin-valves that were investigated in [2]. Power spectra of the various oscillation regimes obtained (depending on applied current) are presented. Finally, in section IV we discuss our findings in comparison with experiments and macrospin simulations of the Slonczewski model, equation (2).

II. Numerical scheme

Let $\vec{g} := \gamma\mu_0 \vec{H}_{eff}/(1+\alpha^2)$, then the system (1), (3) can be written as

$$\partial_t \begin{pmatrix} \vec{m} \\ \vec{s} \end{pmatrix} = \begin{pmatrix} -\vec{m} \times \vec{g} - \alpha \vec{m} \times (\vec{m} \times \vec{g}) \\ D\Delta\vec{s} - \frac{\vec{s}}{\tau} - \frac{J_{ex}}{\hbar} \vec{s} \times \vec{m} \end{pmatrix} =: A(\vec{m}, \vec{s}) \tag{6}$$

where we defined the non-linear operator A. This operator is split into four parts, $A = A_1 + A_2 + A_3 + A_4$, which read

$$A_1(\vec{m}, \vec{s}) := \begin{pmatrix} 0 \\ D\Delta\vec{s} - \frac{\vec{s}}{\tau} - \frac{J_{ex}}{\hbar} \vec{s} \times \vec{m} \end{pmatrix} \tag{7}$$

$$A_2(\vec{m}, \vec{s}) := \begin{pmatrix} -\alpha \vec{m} \times [\vec{m} \times \vec{g}] \\ 0 \end{pmatrix} \tag{8}$$

$$A_3(\vec{m}, \vec{s}) := \begin{pmatrix} -\vec{m} \times \left[\vec{g} - \frac{2\gamma A_{ex}}{M_s(1+\alpha^2)} \Delta\vec{m} \right] \\ 0 \end{pmatrix} \tag{9}$$

$$A_4(\vec{m}, \vec{s}) := \begin{pmatrix} -\vec{m} \times \left[\frac{2\gamma A_{ex}}{M_s(1+\alpha^2)} \Delta\vec{m} \right] \\ 0 \end{pmatrix} \tag{10}$$

In our finite-difference scheme, let $n\Delta t$ denote the discrete moments in time, Δt being the time step. Applying Strang operator splitting [12] to (7)-(10) we obtain the expression

$$(\vec{m}^{n+1}, \vec{s}^{n+1}) = A_1^{\frac{1}{2}} A_2^{\frac{1}{2}} A_3^{\frac{1}{2}} A_4^{1} A_3^{\frac{1}{2}} A_2^{\frac{1}{2}} A_1^{\frac{1}{2}} (\vec{m}^n, \vec{s}^n) \tag{11}$$

Here, $A_i^l(\vec{m}^n, \vec{s}^n)$ denotes an advancement in time of $(\vec{m}^n, \vec{s}^n)$ by $l\Delta t$ by solving a discretized form of the equation $\partial_t(\vec{m}, \vec{s}) = A_i(\vec{m}, \vec{s})$. The operator A_1 is treated with a Crank-Nicolson scheme that is second order in space. The appearing linear system is solved by Gauss-Seidel iteration and we use the fact that the solution to the equation $\vec{x} + \vec{x} \times \vec{a} = \vec{y}$, where $\vec{x}, \vec{a}, \vec{y} \in \mathbb{R}^3$, is given by

$$\vec{x} = \frac{\vec{y} + (\vec{a} \cdot \vec{y})\vec{a} + \vec{a} \times \vec{y}}{1 + |\vec{a}|^2} \tag{12}$$

The damping operator A_2 is treated with a scheme developed in a work by E et al. [13]. For the operator A_3, denoting the expression in the square brackets in (9) by $f(\vec{m}, \vec{s})$, we implement a norm-conserving Crank-Nicolson scheme,

$$\frac{\vec{m}^{**} - \vec{m}^*}{l\Delta t} = -\frac{\vec{m}^{**} + \vec{m}^*}{2} \times f(\vec{m}^*, \vec{s}^*) \tag{13}$$

which is linear in $\vec{m}^{**}$ and is solved by Gauss-Seidel iteration using (12). In case of the operator A_4 we treat the Laplace term implicitly and linearize as follows,

$$\frac{\vec{m}_k^{**} - \vec{m}_k^*}{l\Delta t} = -\frac{\vec{m}_k^{**} + \vec{m}_k^*}{2} \times \frac{\vec{m}_{k+1}^{**} - 2\vec{m}_k^{**} + \vec{m}_{k-1}^{**}}{\Delta x^2} =$$

$$= -\frac{\vec{m}_k^{**} + \vec{m}_k^*}{2} \times \frac{\vec{m}_{k+1}^{**} + 2\vec{m}_k^* + \vec{m}_{k-1}^{**}}{\Delta x^2} \tag{14}$$

Here, k stands for the spatial index and Δx denotes the grid spacing. The system (14) is solved by Gauss-Seidel iteration using (12).

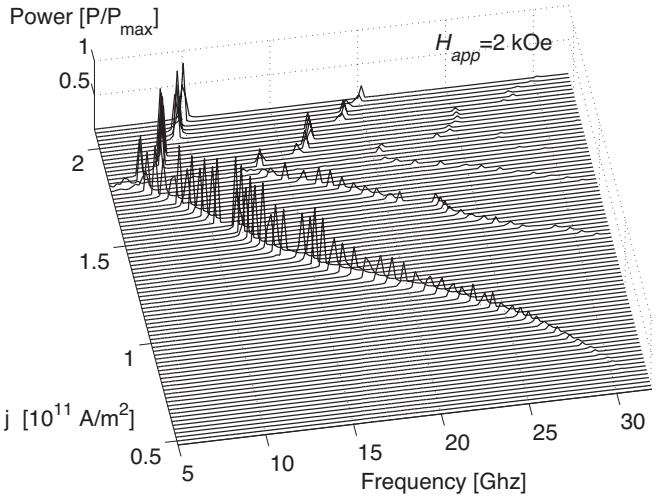


Fig. 1: Simulated power spectra of magnetic oscillations in the investigated spin valve for different current densities j. P_{max} stands for the largest of all observed peaks.

III. Simulation of spin-valve under current

We simulate the spin transfer-torque in a four layer structure that reflects the experimental setup of [2]. The layer

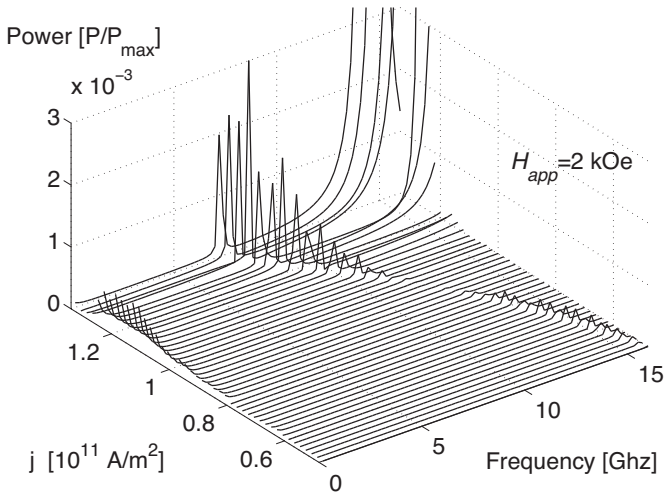
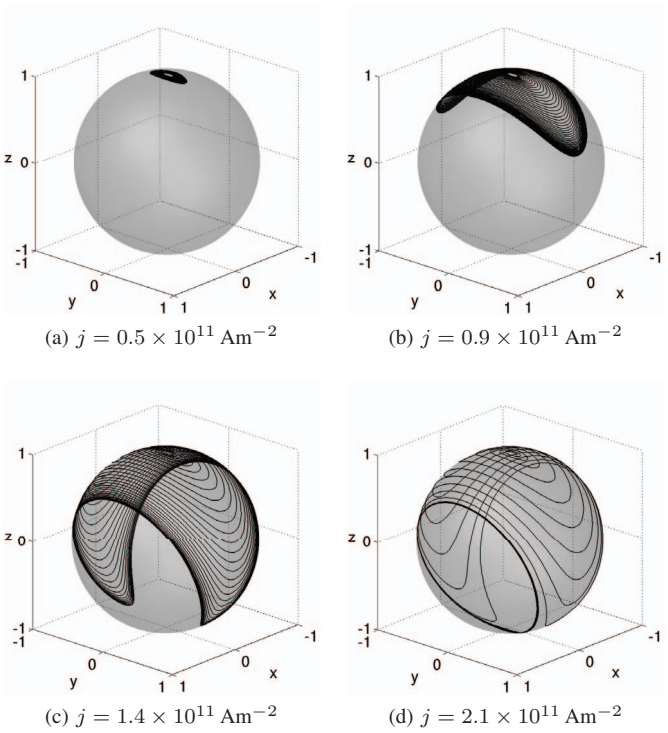


Fig. 2: Simulated power spectra for current densities $j \in [0.48, 1.34] \times 10^{11}\,\mathrm{Am}^{-2}$ in the range of 0-16 Ghz.



(a) $j = 0.5 \times 10^{11}\,\mathrm{Am}^{-2}$ (b) $j = 0.9 \times 10^{11}\,\mathrm{Am}^{-2}$

(c) $j = 1.4 \times 10^{11}\,\mathrm{Am}^{-2}$ (d) $j = 2.1 \times 10^{11}\,\mathrm{Am}^{-2}$

Fig. 3: Obtained oscillation regimes of the mean value $\hat{\vec{m}}(t)$ in the thin FM layer: a) small angle precession, b) large angle precession, c) clamshell orbit, d) out-of-plane precession.

thicknesses are 40 nm FM / 10 nm NM / 3 nm FM / 3 μm NM. Current flows in the x-direction, where x=0 denotes the interface between an electrode and the 40 nm FM layer (F_F), and $\vec{s}(x{=}0, t) = \vec{s}_{inj}(t)$, i.e., the Dirichlet condition is allowed to change in time with the direction of $\vec{m}_F$, see eq. (5). In this setup, the dynamics inflicted on the thick layer magnetization have been found to be minor in the investigated parameter range. A time-independent vector $\vec{s}_{inj}$ does not account for a correct physical picture and changes the results drastically, causing the dynamics of $\vec{m}_F$ to dominate over those in the thin FM layer. The number of grid points in the respective layers is: 32 / 16 / 16 / 64. Further refinement did not cause a change in the results. The easy axis in the thick FM layer is assumed to be in the z-direction and the one in the thin FM layer is chosen to be tilted by 5° to that axis. In the FM layers, we use parameters associated to Cobalt [2], [7], $K_u = 2.41 \times 10^4\,\mathrm{Jm}^{-3}$, $M_s = 8 \times 10^5\,\mathrm{Am}^{-1}$, $A_{ex} = 2 \times 10^{-11}\,\mathrm{Jm}^{-1}$, $\tau = 10^{-12}\,\mathrm{s}$, $\alpha = 0.02$, $D = 10^{-3}\,\mathrm{m}^2\mathrm{s}^{-1}$ and $J_{ex} = 0.1\,\mathrm{eV}$ [8]. In the NM layers we use $D = 10^{-3}\,\mathrm{m}^2\mathrm{s}^{-1}$ and $\tau = 10^{-10}\,\mathrm{s}$. Homogenous Neumann conditions are applied on boundaries for the Landau-Lifshitz equation in each FM layer. Considering the spin-diffusion equation, the boundary/interface conditions discussed in section I are implemented.

In all simulations, a magnetic field $|\vec{H}_{app}| = 2\,\mathrm{kOe}$ was applied in the positive z-direction. Thus, the intitial state of the spin valve is that the magnetizations of both FM layers are almost parallel, $\vec{m}_F$ being perfectly aligned with $\vec{H}_{app}$ and $\vec{m}$ of the thin layer slightly tilted. We then inject a positive current, which, according to equation (5), leads to an $\vec{s}_{inj}$ that is antiparallel to $\vec{m}_F$. The spin density $\vec{s}$ will thus have a small perpendicular component to $\vec{m}$ in the thin FM layer, inflicting the so-called spin-transfer torque. At sufficiently large currents, one observes magnetic oscillations in different regimes (see below) in the thin FM layer. Note that if the easy axis of the thin FM layer would point in the z-direction too, no torque would occur in the zero-temperature ZLF-model studied here. Besides, the intra-layer exchange coupling in the thin FM layer is so strong that its magnetization distribution $\vec{m}(x, t)$ stays almost uniform for all t. In the thick FM layer, $\vec{m}_F(x, t)$ does not stay uniform but shows only very small deviations from $+\vec{z}$ (up to 3°) in the course of a simulation. In all simulations, a time step $\Delta t = 10^{-13}\,\mathrm{s}$ was used, smaller time steps did not lead to a change in the results.

To analyse our simulations, we assume that the deviation of the electrical resistance in a spin valve from its value in the parallel configuration is $\Delta R = \Delta R_{max}(1 - \hat{\vec{m}}_F \cdot \hat{\vec{m}})/2$ [7], where $\hat{\vec{m}}_F \cdot \hat{\vec{m}}$ denotes the dot product of the spatial mean values of the magnetizations in the two FM layers. Power spectra of the magnetic oscillations in the thin layer are obtained by performing a discrete Fourier transform of the simulated signals $\Delta R(t)$ (we use 5000 data points that are spaced by $\Delta t = 10^{-12}\,\mathrm{s}$) and by plotting the squared norm of the Fourier coefficients over the frequency.

Figure 1 shows the power spectra for current densities in the interval $j \in [0.48, 2.10] \times 10^{11}\,\mathrm{Am}^{-2}$. The dominant peaks are the ones corresponding to $2f_0$, i.e., two times the actual oscillation frequency. They start to emerge at around $j = 0.6 \times 10^{11}\,\mathrm{Am}^{-2}$ at $f \approx 30\,\mathrm{Ghz}$ and shift down in frequency with increasing current. At currents larger than $j = 1.4 \times 10^{11}\,\mathrm{Am}^{-2}$, higher harmonics ($4f_0$, $6f_0$) emerge too. The power of the odd harmonics (f_0, $3f_0$, etc.) is three to five orders of magnitude smaller than the one of $2f_0$,

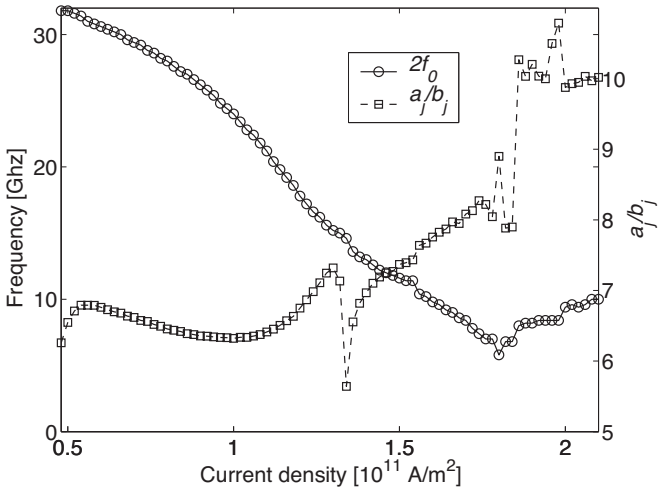


Fig. 4: Simulation results of two times the fundamental oscillation frequency f_0 and the ratio a_j/b_j as a function of current density j.

as can be seen in Figure 2, where power spectra in the intervals $j \in [0.48, 1.34] \times 10^{11}\,\mathrm{Am}^{-2}$ and $f \in [0, 16]\,\mathrm{Ghz}$ are depicted. Oscillations start at a frequency $f_0 = 16\,\mathrm{Ghz}$ for $j = 0.48 \times 10^{11}\,\mathrm{Am}^{-2}$, then f_0 diminishes with increasing current before it emerges again at frequencies lower than 10 Ghz at about two orders of magnitude more powerful. During this transition, we observe a low-frequency background.

We refer to [7] for a detailed interpretation of the obtained power spectra. The main reason for the occurrence of different harmonics is that $\hat{\vec{m}}$ moves along elliptical trajectories that are not symmetric with respect to the z-axis, as can be seen in Figure 3 where the different simulated oscillation regimes are depicted. We found a) small angle precessions, b) large angle precessions, c) clamshell orbits and d) out-of-plane precessions.

As derived by Zhang et al. [8], the effect of adding the $\vec{s}$-term to the effective field, equation (4), can be expressed in compact form by augmenting the Landau-Lifshitz equation by two terms,

$$\partial_t \vec{m}\Big|_{ZLF} = a_j \vec{m} \times (\vec{m} \times \vec{m}_F) + b_j \vec{m} \times \vec{m}_F \qquad (15)$$

This expression differs from the Slonczewski torque term (2) by the second term on the right-hand-side, the so-called effective field term. In our simulations, we determined the coefficients $a_j(x,t)$ and $b_j(x,t)$ in the thin FM layer, integrated them over the thin layer domain and then calculated the ratio of the time mean of these integrals. Results are depicted in Figure 4 for different current densities, along with the corresponding frequencies $2f_0$. The ratio a_j/b_j is found to be roughly 7 for small/large angle precessions and around 10 for out of plane precessions.

IV. Discussion

As far as f_0 is concerned (Figure 2), our results show good qualitative and quantitative agreement with the experimental findings in [2]. However, the much stronger peaks of $2f_0$ (Figure 1) were not reported there, which is quite surprising. The different oscillation regimes (Figure 3) have been reported in macrospin simulations [5] with the Slonczewski spin-torque model (2). The similarity to the ZLF-model is understood by looking at the ratio a_j/b_j (Figure 4), which is between 6 and 10 in our simulations. An experimental value of 5.3 is reported by Zimmler et al. [14] for a 3 nm Cobalt layer.

V. Conclusion

We showed that the diffusive exchange-torque model (ZLF model) proposed by Zhang et al. [8] represents a legitimate alternative to the ballistic interface torque-model usually used to describe magnetization dynamics in spin valves. For the first time a numerical study of the coupled system Landau-Lifshitz equation / spin-diffusion equation has been carried out using reasonable physical parameters in order to enable comparison with experimental data. The obtained simulation results encourage the study of the ZLF-model in greater detail, especially in 3D geometries.

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