Implementation of a non-equilibrium Green’s function method to calculate
spin-transfer torque

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We present an implementation of the steady state Keldysh approach in a Green’s function multiple
scattering scheme to calculate the non-equilibrium spin density. This density is used to obtain the
spin-transfer torque in junctions showing the magnetoresistance effect. We use our implementation
to study the spin-transfer torque in metallic Co/Cu/Co junctions.

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I. INTRODUCTION

The discovery of the giant magnetoresistance (GMR) effect in metallic spin valves systems1,2 has led to sub-
stantial research in the field of spintronics due to the possible applications including read heads in hard disks,
storage elements in magnetic random access memory (MRAM), and sensors.

An effective method for writing information into the elements is necessary for the application as storage el-
ements in MRAM. In particular, one has to be able to change the magnetic orientation of the ferromagnetic
leads relative to each other. One promising approach is the current induced switching proposed by Slonczewski3
and by Berger.4 A current is driven through the junction and becomes spin polarized in one ferromagnetic lead.
This polarization is conserved going through the spacer layer. When the corresponding angular momentum of
the polarized current is not exactly aligned to the magnetization of the second ferromagnetic lead, the electrons
precess around the magnetic moment of the second magnetic layer. In turn this precession leads to a torque
acting on this magnetization forcing it to rotate. When the current is large enough, the magnetic orientation in
the second layer can be switched. There is also a torque acting on the first ferromagnetic layer, but this layer is
magnetically pinned.

In this paper we present an ab initio calculation of the
spin-transfer torque using a multiple scattering Green’s function scheme. In particular, the non-equilibrium spin
density is calculated using the steady state Keldysh approach (see Sec. II A). This spin density is used to cal-
culate the torque acting on the ferromagnetic layer (see Sec. II B). We conclude by testing our approach through
an application to a Co/Cu/Co system, which has been studied by other authors.5,6

FIG. 1: Division of the junction into three regions. Top: coupled (c) system. Middle: isolated (i) system where the
couplings between the middle region and the leads are set to zero. Bottom: decoupled (d) system where the decoupling is
achieved by introducing the potentials $V^c_L$ and $V^c_R$.

II. METHOD

A. Non-equilibrium spin density

The non-equilibrium Green’s function (NEGF) approach is based on dividing the junction into three re-
gions (see Fig. 1): two semi-infinite unperturbed leads left (L) and right (R) and a middle (M) region (or scat-
tering region). This division allows a description of the effect on the middle region of the semi-infinite leads each
having a different chemical potential. The effect on the middle region can be written in terms of a self-energy of
the left lead $\Sigma_L$ given by the coupling from the middle to the left lead and back

$$\Sigma_L = v_{ML} g_L v_{ML}^\dagger$$

where $g_L$ is the surface Green’s function of the isolated semi-infinite left lead and $v_{ML}$ describes the coupling of
the left lead to the middle region. In an analogous way
one defines the self-energy of the right lead $\Sigma_R$. These self-energies can be interpreted as fluxes of incoming and outgoing electrons at the connection between leads and middle region. Using the self-energy of the left and right lead one can express the spin density matrix in the middle region

$$\rho_M = \frac{i}{2\pi} G_{M,c} \left[ (\Sigma_L - \Sigma_L^\dagger) f_L + (\Sigma_R - \Sigma_R^\dagger) f_R \right] G_{M,c}^\dagger \tag{2}$$

where $G_{M,c}$ is the Green’s function of region $M$ coupled (c) to the semi-infinite leads and $f_L$ and $f_R$ are the distribution functions of the left and right lead. All quantities in Eq. (2) are energy dependent. The self-energy can be used to relate the coupled (c) and isolated (i) Green’s functions of the middle region via a Dyson equation

$$G_{M,c} = G_{M,i} + G_{M,i} (\Sigma_L + \Sigma_R) G_{M,c}. \tag{3}$$

This equation is based on the assumption that the self-energies can be added, which is true if the leads are well separated and their interaction can be neglected.

Our approach for calculating the self-energy with a Korringa Kohn Rostoker (KKR) multiple scattering scheme is based on the approach due to Henk et al.,2 following the work by Pendry et al.2 Here we sketch this idea and highlight the basic assumptions which are necessary.

For the calculation of the self-energy using Eq. (1), one needs to know the coupling between the lead and the middle region. In contrast to, e.g., tight binding approaches this coupling is not directly accessible within the KKR scheme because one calculates the Green’s function of a system by a Dyson equation. Hence to obtain the coupling, one has to invert the Green’s function. The alternate approach we use is to introduce decoupling potentials $V_L^d$ and $V_R^d$ (see Fig. 1 bottom) which decouple the middle region from the leads using finite barriers. In the following we show that one can define a self-energy using $V^d$ and the Green’s function $G_d$ of the decoupled system. The Green’s functions of the infinite systems (coupled and decoupled) can be related by the Dyson equation

$$G_c = G_d - G_d \left( V_L^d + V_R^d \right) G_c. \tag{4}$$

Inserting this equation once in itself and using the assumptions (written schematically)

$$G_d \left( V_L^d + V_R^d \right) G_d \ll G_d \left( V_L^d + V_R^d \right) G_d \left( V_L^d + V_R^d \right) G_c \tag{5}$$

and

$$G_d \left( V_L^d G_d V_L^d + V_R^d G_d V_R^d \right) G_c \gg G_d \left( V_L^d G_d V_R^d + V_R^d G_d V_L^d \right) G_c \tag{6}$$

one can identify the self-energies by comparing the result to Eqs. (1) and (3)

$$\Sigma_L = V_L^d G_d V_L^d \text{ and } \Sigma_R = V_R^d G_d V_R^d. \tag{7}$$

Assumptions (1) and (6) are necessary because $V_L^d$ and $V_R^d$ are local potentials whereas $V_{LM}$ in Eq. (1) is a coupling. Assumption (4) is fulfilled if $(V_L^d + V_R^d) G_c >> 1$ which one assures by choosing an appropriately high $V^d$.

Assumption (3) is that the self-energies of the right and left lead can be added. This is fulfilled if the leads are well separated because the elements of $G_d$ relating the left and the right lead decay exponentially with respect to the thickness of the decoupling potential.

By comparing Eqs. (1) and (7) the role of $G_d$ is the role of the surface Green’s function of the isolated leads. Therefore, one can also set the whole middle region to the potential $V^d$ when calculating $G_d$. For details of the implementation using the KKR basis set see Ref. 8.

For the present work, we generalize the method to non-collinear magnetizations based on Ref. 11.

**B. Spin-transfer torque**

From the non-equilibrium Green’s function for a non-collinear magnetization described in the previous section, it is straightforward to compute the spin-transfer torque. In linear response, the spin torque $\vec{\tau}$ per current $I$ on layer $i$ can be expressed by (see Haney et al.5)

$$\frac{\tau}{T} = 2\pi \frac{\mu_B}{e} \int d\vec{k} \| \sum_{l} \vec{\Delta}_l \times \vec{m}_l^T(\vec{k}_l) \|rac{1}{f(k_l)T(k_l)} \tag{8}$$

where $\vec{\Delta}_l$ are the matrix elements of the exchange field along the magnetization axis of the layer $i$ expanded into spherical harmonics with $l$ being the angular momentum. $\vec{m}_l^T$ is the magnetic moment of the electrons contributing to the transport and is calculated from the non-equilibrium spin density matrix at the Fermi level $E_F$ using Eq. (2)

$$\rho_{lr} = \frac{i}{2\pi} G_c(E_F) \left( \Sigma_L(E_F) - \Sigma_L^\dagger(E_F) \right) G_c^\dagger(E_F) \tag{9}$$

taking into account that the electronic states at $E_F$ are occupied only in one lead. The transmission probability $T$ is calculated by

$$T = \text{Tr} \left[ \left( \Sigma_L - \Sigma_L^\dagger \right) G \left( \Sigma_R - \Sigma_R^\dagger \right) G^\dagger \right]. \tag{10}$$

where the trace is over the spin index and the basis set expansion. Due to the in-plane translational invariance of the junctions one can label the states by the wave vector $k_l$ and all quantities in Eqs. (9) and (10) depend on $k_l$. To get the total values one has to integrate over the 2D Brillouin zone.

**III. APPLICATION TO Co/Cu/Co**

In this section we test our approach by applying it to a Co/Cu/Co system. In particular, we consider the dependence of the torque on the angle between the two magnetizations of the ferromagnetic leads. For this purpose,
we use the same structure used in Ref. [3] consisting of a semi-infinite Co, 9 monolayers Cu, 15 monolayers Co, and semi-infinite Cu. The lattice constant is 0.361 nm. Fig. 2 shows the dependence of the conductance $g$ on the relative angle $\theta$ between the magnetizations of the Co layers. We find excellent agreement with Ref. [5] and a GMR ratio $(g(0^\circ) - g(180^\circ)) / g(180^\circ) = 47 \%$.

Fig. 3 shows the in-plane torque $\tau_\parallel$ and the out-of-plane torque $\tau_\perp$ as a function of the angle $\theta$ for two different $k_\parallel$ point samples. The out-of-plane torque has two contributions: one from the right going states that are occupied and have no left going counterparts, and the other from states below both chemical potentials in which both left and right going states are occupied. The latter contribution requires integration over energy as well as parallel wave vector. However, the usage of a complex energy contour makes it easier to converge. For the former contribution one cannot use a complex energy because only right going states are occupied. Therefore, to test our method against previous calculations and to test the $k$-point convergence, we consider only this contribution to the out-of-plane torque in the following. The dependence of $\tau_\parallel$ on $\theta$ is the same for both $k_\parallel$ samplings and is in good agreement to Ref. [3]. In contrast, $\tau_\perp$ shows rapid oscillations as a function of $\theta$ for the $k_\parallel$ sampling using 40 000 $k_\parallel$ points. A similar dependence was observed in Ref. [3]. However, a significantly larger $k_\parallel$ point sample leads to an almost smooth dependence of $\tau_\perp$ on $\theta$.

Due to the drastic change in $\tau_\perp$ from increasing the number of $k_\parallel$ points, we test the convergence of the in-plane torque $\tau_\parallel$ and the out-of-plane torque $\tau_\perp$ for a fixed angle $\theta = 60^\circ$ as a function of the number of $k_\parallel$ points (see Fig. 4). For $\tau_\parallel$ the convergence is fast and a relatively low number of $k_\parallel$ points is sufficient. On the other hand $\tau_\perp$ is very sensitive to the number of $k_\parallel$ points and a large number is necessary to get convergence. The slow convergence results from the presence of short period oscillations at the corners of the 2D Brillouin zone which require a very fine mesh. Therefore, the rapid oscillations in $\tau_\perp$ as a function of angle found in Ref. [3] disappear for fully converged $k_\parallel$ point samples.

**IV. CONCLUSION**

We present a method to calculate the spin-transfer torque within a screened KKR scheme by calculating the non-equilibrium spin density using the steady state Keldysh approach. The in-plane torque in the Co/Cu/Co junctions is robust with respect to the $k_\parallel$ point sampling but the out-of-plane torque converges slowly with respect to the number of $k_\parallel$ points. The reason is that there are short period oscillations at the edges of the 2D Brillouin zone. These oscillation require a very fine $k_\parallel$ point mesh to get the correct value for the integral. Then both components of the torque are a smooth function of the angle but with maxima at different angles.
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1 M. Baibich, J. Broto, A. Fert, P. N. V. Dau, F. Petro, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. 61, 2472 (1988).
2 G. Binasch, P. Grünberg, F. Saurenbach, and W. Zinn, Phys. Rev. B 39, 4828 (1989).
3 J.C. Slonczewski, J. Magn. Magn. Mater. 159, L1 (1996).
4 L. Berger, Phys. Rev. B 54, 9353 (1996).
5 P.M. Haney, D. Waldron, R.A. Duine, A.S. Núñez, H. Guo, and A.H. MacDonald, Phys. Rev. B 76, 024404 (2007).
6 D. M. Edwards, F. Federici, J. Mathon, and A. Umerski, Phys. Rev. B 71, 054407 (2005).
7 S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press (1999).
8 J. Henk, A. Ernst, K.K. Saha, and P. Bruno, J. Phys.: Condens. Matter 18, 2601 (2006).
9 J.B. Pendry, A.B. Prte, and B.C.H. Krutzen, J. Phys.: Condens. Matter 3, 4313 (1991).
10 B. Yu, Yavorsky and I. Mertig, Phys. Rev. B 74, 174402 (2006).