

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 systems^{1,2} has led to substantial 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 elements 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 calculate 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}

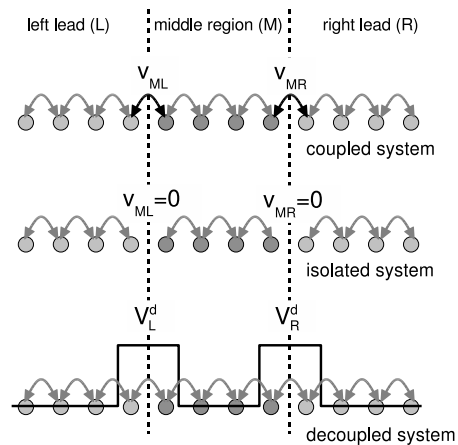


FIG. 1: Division of the junction into three regions. Top: coupled (c) system. Middle: isolated (i) system where the couplings between the middle region and the leads are set to zero. Bottom: decoupled (d) system where the decoupling is achieved by introducing the potentials V_L^d and V_R^d .

II. METHOD

A. Non-equilibrium spin density

The non-equilibrium Green's function (NEGF) approach is based on dividing the junction into three regions (see Fig. 1): two semi-infinite unperturbed leads left (L) and right (R) and a middle (M) region (or scattering 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 Σ_L given by the coupling from the middle to the left lead and back

$$\Sigma_L = v_{ML} g_L v_{ML}^\dagger \quad (1)$$

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 Σ_R . These self-energies can be interpreted as fluxes of incoming and outgoing electrons at the connection between leads and middle region.⁷ Using the self-energy of the left and right lead one can express the spin density matrix in the middle region

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

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 the distribution functions of the left and right lead.⁷ 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

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

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.*⁸, following the work by Pendry *et al.*⁹ 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 approaches⁶ 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

$$G_c = G_d - G_d (V_L^d + V_R^d) G_c . \quad (4)$$

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

$$G_d (V_L^d + V_R^d) G_d \ll G_d (V_L^d + V_R^d) G_d (V_L^d + V_R^d) G_c \quad (5)$$

and

$$G_d (V_L^d G_d V_L^d + V_R^d G_d V_R^d) G_c \gg G_d (V_L^d G_d V_R^d + V_R^d G_d V_L^d) G_c \quad (6)$$

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

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

Assumptions (5) 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 (5) is fulfilled if $(V_L^d + V_R^d) G_c \gg 1$ which one assures by choosing an appropriately high V^d . Assumption (6) 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. 10.

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)

$$\frac{\vec{\tau}}{I} = 2\pi \frac{\mu_B}{e} \frac{\int d\mathbf{k}_\parallel \sum_l \vec{\Delta}_l \times \vec{m}_l^{tr}(\mathbf{k}_\parallel)}{\int d\mathbf{k}_\parallel T(\mathbf{k}_\parallel)} \quad (8)$$

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^{tr} 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)

$$\rho^{tr} = \frac{i}{2\pi} G_c(E_F) \left(\Sigma_L(E_F) - \Sigma_L^\dagger(E_F) \right) G_c^\dagger(E_F) \quad (9)$$

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

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

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 \mathbf{k}_\parallel and all quantities in Eqs. (9) and (10) depend on \mathbf{k}_\parallel . 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,

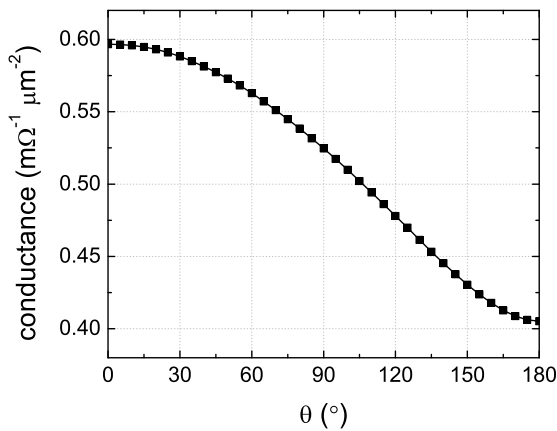


FIG. 2: Conductance of the Co/Cu/Co/Cu spin valve as a function of the relative angle between both magnetization of the ferromagnetic layers.

we use the same structure used in Ref. 5 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 θ 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 τ_{\parallel} and the out-of-plane torque τ_{\perp} as a function of the angle θ for two different \mathbf{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 can not use a complex energy because only right going states are occupied. Therefore, to test our method against previous calculations and to test the \mathbf{k} -point convergence, we consider only this contribution to the out-of-plane torque in the following. The dependence of τ_{\parallel} on θ is the same for both \mathbf{k}_{\parallel} samplings and is in good agreement to Ref. 5. In contrast, τ_{\perp} shows rapid oscillations as a function of θ for the \mathbf{k}_{\parallel} sampling using 40 000 \mathbf{k}_{\parallel} points. A similar dependence was observed in Ref. 5. However, a significantly larger \mathbf{k}_{\parallel} point sample leads to an almost smooth dependence of τ_{\perp} on θ .

Due to the drastic change in τ_{\perp} from increasing the number of \mathbf{k}_{\parallel} points, we test the convergence of the in-plane torque τ_{\parallel} and the out-of-plane torque τ_{\perp} for a fixed angle $\theta = 60^\circ$ as a function of the number of \mathbf{k}_{\parallel} points (see Fig. 4). For τ_{\parallel} the convergence is fast and a relatively low number of \mathbf{k}_{\parallel} points is sufficient. On the other hand τ_{\perp} is very sensitive to the number of \mathbf{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

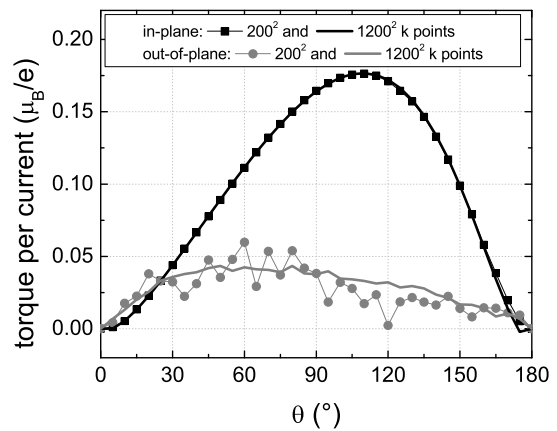


FIG. 3: Torque per current as a function of the relative angle between both magnetizations of the ferromagnetic layers for two different numbers of \mathbf{k}_{\parallel} points in the whole 2D Brillouin zone.

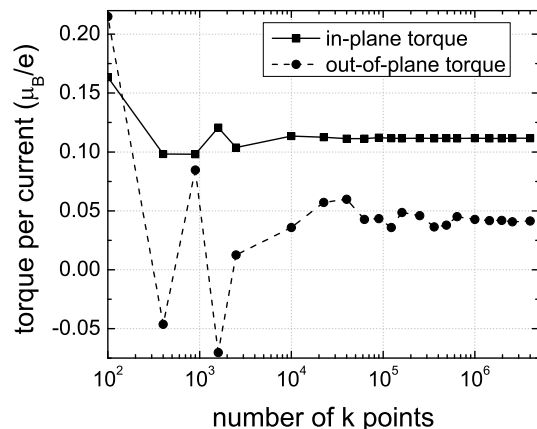


FIG. 4: Convergence test for the torque with respect to the number of \mathbf{k}_{\parallel} points in the whole 2D Brillouin zone.

require a very fine mesh. Therefore, the rapid oscillations in τ_{\perp} as a function of angle found in Ref. 5 disappear for fully converged \mathbf{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 \mathbf{k}_{\parallel} point sampling but the out-of-plane torque converges slowly with respect to the number of \mathbf{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 \mathbf{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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