# **Landauer theory of ballistic torkances in noncollinear spin valves**

K. Carva<sup>1,2[,\\*](#page-4-0)</sup> and I. Turek<sup>1[,†](#page-4-1)</sup>

1 *Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Charles University, Ke Karlovu 5,*

*CZ-12116 Prague 2, Czech Republic*

<sup>2</sup>*Department of Physics and Materials Science, Uppsala University, P.O. Box 530, SE-75121 Uppsala, Sweden*

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We present a theory of voltage-induced spin-transfer torques in ballistic noncollinear spin valves. The torkance on one ferromagnetic layer is expressed in terms of scattering coefficients of the whole spin valve, in analogy to the Landauer conductance formula. The theory is applied to  $Co/Cu/Ni(001)$ -based systems where long-range oscillations of the Ni torkance as a function of Ni thickness are predicted. The oscillations represent a novel quantum size effect due to the noncollinear magnetic structure. The oscillatory behavior of the torkance contrasts a thickness-independent trend of the conductance.

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# **I. INTRODUCTION**

The prediction<sup>1[,2](#page-4-3)</sup> and realization<sup>3[,4](#page-4-5)</sup> of current-induced switching of magnetization direction in epitaxial magnetic multilayers stimulated huge research activity related to highdensity writing of information. The simplest systems for this purpose are spin valves NM/FM1/NM/FM2/NM with two ferromagnetic (FM) layers (FM1 and FM2) separated by a nonmagnetic (NM) spacer layer and attached to semi-infinite NM metallic leads. The electric current perpendicular to the layers becomes spin polarized on passing the FM1 layer with a fixed magnetization direction. In noncollinear spin valves, subsequent reflection and transmission of spin-polarized electrons at the FM2 layer result in a spin torque acting on its magnetization the direction of which can thus be changed. Majority of existing experimental and theoretical studies of these spin-transfer torques refer to a diffusive regime of electron transport in metallic systems, see Ref. [5](#page-4-6) for a review.

Magnetic tunnel junctions with the NM spacer layer replaced by an insulating barrier have attracted attention only very recently; in these systems voltage-driven spin-transfer torques<sup>6</sup> as well as effects of finite bias<sup>7[,8](#page-4-9)</sup> can be studied. The concept of torkance, defined in the small-bias limit as a ratio of the spin-transfer torque and the applied voltage, $6$  represents an analogy to the conductance. It becomes important also for all-metallic spin valves with ultrathin layers<sup>9[,10](#page-5-1)</sup> where a ballistic regime of electron transport can be realized.

The latter regime is amenable to fully microscopic, quantum-mechanical treatments. All existing theoretical ap-proaches to the torkance, both on model<sup>7,[9,](#page-5-0)[11](#page-5-2)[,12](#page-5-3)</sup> and *ab levels, are based on a linear response of various* local quantities inside the spin valve to the applied bias. The local quantities used range from scattering coefficients of the individual layers<sup>12</sup> over local spin currents<sup>9</sup> to site- and orbital-resolved elements of a one-particle density matrix[.11](#page-5-2) These methods contrast the well-known Landauer picture of the ballistic conductance $13,14$  $13,14$  which employs only transmission coefficients between propagating states of the two leads.

In this paper, we present an alternative theoretical approach to ballistic torkances that yields a result similar to the Landauer conductance formula, i.e., we relate the torkance to scattering coefficients of the whole spin valve. This unified theory of both transport quantities is used to discuss a special consequence of ballistic transport, namely, a predicted oscillatory dependence on Ni thickness in a Cu/Co/Cu/Ni/  $Cu(001)$  system. The presented study reveals a relation between the torkance and the properties of individual parts of the spin valve which might be relevant for design of new systems.

#### **II. THEORY**

### **A. Model of the spin valve**

Our approach is based on an effective one-electron Hamiltonian of the NM/FM1/NM/FM2/NM system

$$
H = H_0 + \gamma_1 \mathbf{n}_1 \cdot \boldsymbol{\sigma} + \gamma_2 \mathbf{n}_2 \cdot \boldsymbol{\sigma},\tag{1}
$$

<span id="page-0-0"></span>where  $H_0$  comprises all spin-independent terms,  $\gamma_1 = \gamma_1(\mathbf{r})$ and  $\gamma_2 = \gamma_2(\mathbf{r})$  denote magnitudes of exchange splittings of the FM1 and FM2 layers, respectively,  $n_1$  and  $n_2$  are unit vectors parallel to directions of the exchange splittings, and the  $\sigma = (\sigma_x, \sigma_y, \sigma_z)$  are the Pauli spin matrices. The angle between  $\mathbf{n}_1$  and  $\mathbf{n}_2$  is denoted as  $\theta$ . The spin torque  $\tau$  is defined as time derivative of the electron spin, represented (in units of Bohr magneton) by operator  $\sigma$ . This yields (with  $\hbar$ =1) the total spin torque as

$$
\boldsymbol{\tau} = -\mathrm{i}[\boldsymbol{\sigma}, H] = \boldsymbol{\tau}_1 + \boldsymbol{\tau}_2,\tag{2}
$$

where the quantities

$$
\tau_j = 2\gamma_j \mathbf{n}_j \times \boldsymbol{\sigma}, \quad j = 1, 2,
$$
 (3)

can be interpreted as torques experienced by the two FM layers. Obviously, the torque  $\tau_j$  is perpendicular to the vector **n**<sub>*j*</sub> and it can thus be decomposed with respect to the common plane of the two magnetization vectors into its in-plane  $(\tau_{j\parallel})$  and out-of-plane  $(\tau_{j\perp})$  components, see Fig. [1](#page-1-0) for  $j=2$ . The unit normal vector of the plane is given by  $v = n_1$  $\times$  **n**<sub>2</sub>/sin  $\theta$ .

#### **B. In-plane torkance**

<span id="page-0-1"></span>The basic idea for the in-plane torkance on the FM2 layer rests on the orthogonality relations  $\mathbf{n}_j \cdot \boldsymbol{\tau}_j = 0$ ,  $j = 1, 2$ , from which the size of  $\tau_{2\parallel}$  can be written as

<span id="page-1-0"></span>

FIG. 1. (Color online) The in-plane  $(\tau_{2\parallel})$  and out-of-plane  $(\tau_{2\perp})$ components of the torque  $\tau_2 = \tau_{2\parallel} + \tau_{2\perp}$  experienced by the FM2 layer. For details, see text.

$$
(\mathbf{n}_2 \times \boldsymbol{\nu}) \cdot \boldsymbol{\tau}_2 = \frac{\mathbf{n}_1 \cdot \boldsymbol{\tau}_2}{\sin \theta} = \frac{\mathbf{n}_1 \cdot \boldsymbol{\tau}}{\sin \theta},
$$
(4)

<span id="page-1-1"></span>see Fig. [1.](#page-1-0) The total torque  $\tau$ , being a full time derivative of  $\sigma$ , in Eq. ([4](#page-1-1)) plays a key role in the following treatment. Our approach applies to systems consisting of the left  $(L)$  and the right  $(R)$  semi-infinite NM leads with an intermediate region  $(I)$  in between; the latter contains both FM layers and the NM spacer of the spin valve. Projection operators on these regions are denoted, respectively, as  $\Pi_{\mathcal{L}}$ ,  $\Pi_{\mathcal{R}}$ , and  $\Pi_{\mathcal{I}}$ ; they are mutually orthogonal and satisfy  $\Pi_{\mathcal{L}} + \Pi_{\mathcal{I}} + \Pi_{\mathcal{R}} = 1$ . The Hamiltonian  $(1)$  $(1)$  $(1)$  is assumed to be short ranged (tight binding), not coupling the two leads, i.e.,  $\Pi_L H \Pi_R = 0$ . The leads are in thermodynamic equilibrium at zero temperature. A general linear-response theory can be formulated for a Hermitean operator  $Q = Q^+$  that is local, i.e., not coupling neighboring parts of the system, so that  $Q = \Pi_{\mathcal{L}} Q \Pi_{\mathcal{L}} + \Pi_{\mathcal{I}} Q \Pi_{\mathcal{I}}$  $+\Pi_{\mathcal{R}}Q\Pi_{\mathcal{R}}$ . Its time derivative

$$
D = -i[Q, H] \tag{5}
$$

<span id="page-1-3"></span>is assumed to be localized in *I*, i.e.,  $D = \prod_{\mathcal{I}} D \prod_{\mathcal{I}}$ . These properties make it possible to remove the semi-infinite leads from the formalism.

The resulting response coefficient describing the change  $\delta\overline{D}$  in the thermodynamic average of the quantity *D* due to an infinitesimal variation  $\delta \mu_c$  in the chemical potential (Fermi energy) of the  $\mathcal L$  lead is given by

<span id="page-1-2"></span>
$$
\frac{\delta \bar{D}}{\delta \mu_{\mathcal{L}}} = \frac{1}{2\pi} \text{Tr} \{ Q(\Gamma_{\mathcal{R}} G^{\prime} \Gamma_{\mathcal{L}} G^a - \Gamma_{\mathcal{L}} G^{\prime} \Gamma_{\mathcal{R}} G^a) \},\tag{6}
$$

where the trace (Tr) and all symbols on the rhs are defined on the Hilbert space of the intermediate region  $I$ , in particular the *Q* in Eq. ([6](#page-1-2)) abbreviates  $\Pi_{\mathcal{I}}Q\Pi_{\mathcal{I}}$ . The other symbols in Eq. ([6](#page-1-2)) refer to the antihermitean part of the  $\mathcal L$  and  $\mathcal R$  selfenergies,  $\Gamma_{\mathcal{L},\mathcal{R}}(E) = i[\Sigma_{\mathcal{L},\mathcal{R}}^r(E) - \Sigma_{\mathcal{L},\mathcal{R}}^a(E)],$  and to the retarded and advanced propagators

$$
G^{r,a}(E) = [E - H - \Sigma^{r,a}(E)]^{-1},\tag{7}
$$

where  $\Sigma^{r,a}(E) = \Sigma^{r,a}_{\mathcal{L}}(E) + \Sigma^{r,a}_{\mathcal{R}}(E)$  denotes the total self-energy. Omitted energy arguments in Eq.  $(6)$  $(6)$  $(6)$  are equal to the Fermi energy of the equilibrium system  $(E = E_F)$ .

The proof of Eq.  $(6)$  $(6)$  $(6)$  is based on nonequilibrium Green's functions (NGF) for stationary states<sup>15</sup> and it is similar to a previous derivation in Ref. [16.](#page-5-7) The starting point is an expression for the variation in  $\overline{D}$ 

<span id="page-1-4"></span>
$$
\delta \overline{D} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \text{Tr}\{G^a(E)DG^r(E)\delta \Sigma^<(E)\} dE,\tag{8}
$$

where the variation in the lesser part of the self-energy at zero temperature is given by

$$
\delta \Sigma^{<}(E) = \delta (E - E_F) \Gamma_{\mathcal{L}}(E) \delta \mu_{\mathcal{L}}.
$$
 (9)

<span id="page-1-7"></span>The assumed properties of *H*, *Q*, and *D* lead to a commutation rule for the self-energy

$$
[Q, \Sigma_{\mathcal{L}, \mathcal{R}}^{r, a}(E)] = 0,\tag{10}
$$

<span id="page-1-9"></span>which is proved in the Appendix and which in turn yields a relation

$$
G^{a}(E)DG^{r}(E) = i[G^{a}(E)Q - QG^{r}(E)] + G^{a}(E)Q\Gamma(E)G^{r}(E),
$$
\n(11)

where  $\Gamma(E) = i[\Sigma^{r}(E) - \Sigma^{a}(E)] = \Gamma_{\mathcal{L}}(E) + \Gamma_{\mathcal{R}}(E)$ . The result Eq.  $(6)$  $(6)$  $(6)$  follows then from an identity for the spectral density operator

$$
i[Gr(E) - Ga(E)] = Ga(E)\Gamma(E)Gr(E).
$$
 (12)

<span id="page-1-8"></span>Note that the final response coefficient Eq.  $(6)$  $(6)$  $(6)$  obeys a perfect  $\mathcal{L}$ − $\mathcal{R}$  symmetry, i.e.,  $\delta D/\delta \mu_{\mathcal{R}} = -\delta D/\delta \mu_{\mathcal{L}}$ . It should be emphasized that the derived general result Eq. ([6](#page-1-2)) and its perfect L−R symmetry are valid only for operators *D* that can be formulated as a time derivative of a local operator *Q* according to Eq.  $(5)$  $(5)$  $(5)$ . In the present context of spin valves, this is the case of the usual particle conductance and of the in-plane torkance (see below). The out-of-plane torkance requires a different approach based on the more general relation  $(8)$  $(8)$  $(8)$ , see Sec. [II C;](#page-2-0) its symmetry properties for symmetric spin valves were discussed in details, e.g., in Ref. [17.](#page-5-8)

Application of the derived formula  $(6)$  $(6)$  $(6)$  to the transport properties of the spin valves is now straightforward. The usual particle conductance *C* is based on the operator *Q* being a projector on a half-space containing, e.g., the  $R$  lead and an adjacent part of the  $I$  region. This results in the wellknown expression $14$ 

$$
C = \frac{1}{2\pi} \text{Tr}(\Gamma_{\mathcal{R}} G^T \Gamma_{\mathcal{L}} G^a),\tag{13}
$$

<span id="page-1-6"></span>where atomic units  $(e = \hbar = 1)$  are used. The in-plane torkance  $C_{\parallel}$  on FM2 according to Eq. ([4](#page-1-1)) is obtained from  $Q = \mathbf{n}_1 \cdot \boldsymbol{\sigma}$  in Eq. ([6](#page-1-2)). This yields  $C_{\parallel} = C_1 / \sin \theta$ , where

<span id="page-1-5"></span>
$$
C_1 = \frac{1}{2\pi} \text{Tr} \{\mathbf{n}_1 \cdot \boldsymbol{\sigma} (\Gamma_{\mathcal{R}} G^T \Gamma_{\mathcal{L}} G^a - \Gamma_{\mathcal{L}} G^T \Gamma_{\mathcal{R}} G^a) \}.
$$
 (14)

The two terms on rhs can be related to spin fluxes on two sides of the FM2 layer. The expression  $(14)$  $(14)$  $(14)$  represents our

central result. The operators  $\Gamma_{\mathcal{L}}$  and  $\Gamma_{\mathcal{R}}$  are localized in narrow regions at the interfaces  $\mathcal{L}/\mathcal{I}$  and  $\mathcal{I}/\mathcal{R}$ , respectively. The Green's functions (propagators) for points deep inside the spin valve thus enter neither the conductance Eq.  $(13)$  $(13)$  $(13)$  nor the in-plane torkance Eq. ([14](#page-1-5)).

#### **C. Out-of-plane torkance**

<span id="page-2-0"></span>A similar approach for the out-of-plane torkance on the FM2 layer employs an infinitesimal variation  $\delta$ **n**<sub>2</sub> in its magnetization direction due to a variation  $\delta\theta$  in the angle. The FM1 magnetization direction as well as the plane of the two directions  $\mathbf{n}_1$ ,  $\mathbf{n}_2$  remain fixed, i.e.,  $\delta \mathbf{n}_1 = \delta \mathbf{\nu} = 0$ . This leads to  $\delta \mathbf{n}_2 = \mathbf{v} \times \mathbf{n}_2 \delta \theta$  and from ([1](#page-0-0)) also to

$$
H' \equiv \frac{\delta H}{\delta \theta} = \gamma_2 (\nu \times \mathbf{n}_2) \cdot \boldsymbol{\sigma} = \frac{1}{2} \nu \cdot \boldsymbol{\tau}_2 \tag{15}
$$

<span id="page-2-1"></span>so that the size of  $\tau_{2\perp}$  coincides (up to factor of 2) with angular derivative of the effective Hamiltonian *H*. The NGF formulation of the out-of-plane torkance rests on relation ([8](#page-1-4)) applied to the operator  $D=2H'$ , see Eq. ([15](#page-2-1)) with variation in the self-energy  $\delta \Sigma^{\leq}(E)$  due to an infinitesimal variation in the chemical potential  $\delta \mu_{\mathcal{L}}$  given by Eq. ([9](#page-1-7)) and similarly for  $\delta \Sigma^{\leq}(E)$  due to the  $\delta \mu_{\mathcal{R}}$ . This yields then response coefficients  $C_{\mathcal{L}} = \delta \bar{D} / \delta \mu_{\mathcal{L}}$  and  $C_{\mathcal{R}} = \delta \bar{D} / \delta \mu_{\mathcal{R}}$  for the out-of-plane torque with respect to chemical potentials of the  $\mathcal L$  and  $\mathcal R$ leads expressed as

$$
C_{\mathcal{L},\mathcal{R}} = \frac{1}{\pi} \text{Tr}(H' G' \Gamma_{\mathcal{L},\mathcal{R}} G^a). \tag{16}
$$

By employing a simple consequence of Eq.  $(12)$  $(12)$  $(12)$ ,  $G^a = (12)$  $+iG<sup>a</sup>\Gamma$ )*G*<sup>*r*</sup>, cyclic invariance of trace, angular independence of the self-energy of NM leads,  $\Sigma^{r} = \Sigma^{r} = 0$ , and the rule  $G'H'G' = G'$ , the response coefficients can be recast into

$$
C_{\mathcal{L},\mathcal{R}} = \frac{1}{\pi} \text{Tr} \{ G^{\prime \prime} \Gamma_{\mathcal{L},\mathcal{R}} [1 + \mathrm{i} G^a (\Gamma_{\mathcal{L}} + \Gamma_{\mathcal{R}})] \},\tag{17}
$$

which contain again only propagators at points close to the  $\mathcal{L}/\mathcal{I}$  and  $\mathcal{I}/\mathcal{R}$  interfaces, similarly to Eqs. ([13](#page-1-6)) and ([14](#page-1-5)).

The applied bias has to be identified with the difference  $\mu_{\mathcal{L}} - \mu_{\mathcal{R}}$  and the out-of-plane torkance on FM2 is thus given by  $C_{\perp} = (C_{\mathcal{L}} - C_{\mathcal{R}})/2$ . Since the Hamiltonian ([1](#page-0-0)) does not contain spin-orbit interaction, the spin reference system can be chosen such that both unit vectors  $\mathbf{n}_1$  and  $\mathbf{n}_2$  lie in the *x* −*z* plane. This implies that *H* is essentially time-inversion invariant and it can be represented by a symmetric matrix,  $H<sup>T</sup> = H$ ; the related quantities  $G<sup>r,a</sup>$  and  $\Gamma_{\mathcal{L},\mathcal{R}}$  are symmetric as well. As a consequence, the transmissionlike terms in  $C_{\mathcal{L}}$  and  $C_R$  are the same, i.e.,  $Tr(G'T_{\mathcal{L}}G^a\Gamma_R) = Tr(G'T_{\mathcal{R}}G^a\Gamma_{\mathcal{L}})$ . The resulting out-of-plane torkance

<span id="page-2-2"></span>
$$
C_{\perp} = \frac{1}{2\pi} \text{Tr} \{ G^{\prime\prime} [\Gamma_{\mathcal{L}} (1 + \mathrm{i} G^a \Gamma_{\mathcal{L}}) - \Gamma_{\mathcal{R}} (1 + \mathrm{i} G^a \Gamma_{\mathcal{R}}) ] \}
$$
\n(18)

contains thus only reflectionlike terms.

### **D. Landauer formalism**

The Green's function expression for the conductance Eq.  $(13)$  $(13)$  $(13)$  can be translated in the language of scattering theory;<sup>18</sup> the counterparts of the torkances Eqs.  $(14)$  $(14)$  $(14)$  and  $(18)$  $(18)$  $(18)$  are interesting as well. In the present case, propagating states in the  $\mathcal L$  and  $\mathcal R$  lead will be labeled by  $\lambda$  and  $\rho$ , respectively. Moreover, a spin index  $s = \uparrow$ ,  $\downarrow$  has to be used even for NM leads since noncollinearity of the spin valve gives rise to full spin dependence of scattering coefficients.

The conductance Eq.  $(13)$  $(13)$  $(13)$  is given by the Landauer formula  $C = (2\pi)^{-1} \sum_{\lambda \rho s s'} |t_{\rho s',\lambda s}|^2$ , where  $t_{\rho s',\lambda s}$  denotes the transmission coefficient from an incoming state  $\lambda s$  into an outgoing state  $\rho s'$ .<sup>[13](#page-5-4)</sup> The in-plane torkance coefficient Eq. ([14](#page-1-5)) can be written as

$$
C_1 = \frac{1}{2\pi} \sum_{\lambda \rho s s' s''} (\mathbf{n}_1 \cdot \boldsymbol{\sigma})_{s'' s'} (t_{\rho s', \lambda s} t_{\rho s'', \lambda s}^* - t_{\lambda s', \rho s} t_{\lambda s'', \rho s}^*),
$$
\n(19)

whereas the out-of-plane torkance Eq.  $(18)$  $(18)$  $(18)$  can be transformed into

$$
C_{\perp} = \frac{1}{2\pi} \left( \sum_{\lambda s \lambda' s'} r'_{\lambda' s', \lambda s} r^*_{\lambda' s', \lambda s} - \sum_{\rho s \rho' s'} r'_{\rho' s', \rho s} r^*_{\rho' s', \rho s} \right),\tag{20}
$$

where  $r_{\lambda's',\lambda s}(r_{\rho's',\rho s})$  denote reflection coefficients between states of the  $\mathcal{L}(\mathcal{R})$  lead. This result represents analogy to the Landauer formula and it completes the unified theory of conductances and torkances.

## **III. RESULTS FOR Cu/Co/Cu/Ni/Cu(001) AND THEIR DISCUSSION**

The developed formalism allows to study properties of spin valves with ultrathin layers, which is yet an experimentally unexplored area; here we demonstrate its use for understanding unexpected features of *ab initio* results. The results discussed below were obtained using the response of spin currents on both sides of the FM2 layer, $7.9$  implemented within the scalar relativistic tight-binding linear muffin-tin orbital method<sup>19,[20](#page-5-11)</sup> similarly to our previous transport studies[.16,](#page-5-7)[21](#page-5-12) As a case study, spin valves Cu/Co/Cu/Ni/ Cu(001) with face-centered cubic (fcc) structure were chosen. All atomic positions were given by an ideal fcc Co lattice with sharp interfaces between the neighboring FM and NM layers. The spin valves discussed below consist of a Co layer of 5 monolayer (ML) thickness separated by a 10 ML thick Cu spacer from a Ni layer of varying thickness, embedded between two semi-infinite Cu leads. Self-consistent calculations within the local spin-density approximation were performed only for collinear spin valves  $(\theta=0 \text{ or } \theta=\pi)$  while the electronic structure of noncollinear systems was obtained by rotation of the exchange-split potentials of the Co and Ni FM layers. Particular attention has been paid to the convergence of torkances with respect to the number of  $\mathbf{k}_{\parallel}$  vectors sampling the two-dimensional Brillouin zone (BZ) of the system; in agreement with Ref. [22](#page-5-13) we found that reliable

<span id="page-3-0"></span>

FIG. 2. (Color online) Calculated transport coefficients (per interface atom) as functions of Ni thickness: (a) the conductance (C) for three values of the angle  $\theta$  and the in-plane  $(C_{\parallel})$  and out-ofplane  $(C_{\perp})$  Ni torkances for  $\theta = \pi/2$  in spin valves Cu/Co/Cu/Ni/  $Cu(001)$ , (b) the real and imaginary parts of the spin-mixing conductance  $(C^{\text{mix}})$  of Cu/Ni/Cu(001) systems.

values of the out-of-plane torkances require finer meshes than for the in-plane torkances. The presented data were obtained with 6400  $\mathbf{k}_{\parallel}$  points in the whole BZ.

Figure  $2(a)$  $2(a)$  displays the calculated conductances for parallel ( $\theta = 0$ ), antiparallel ( $\theta = \pi$ ), and perpendicular ( $\theta = \pi/2$ ) orientations as well as Ni torkances in the latter case as functions of Ni thickness. The most pronounced feature of the transport coefficients are oscillations with a period of about 12 ML seen in both components of the torkance. These oscillations reflect the perfect ballistic regime of electron transport across the whole spin valve. In addition, they contradict a generally accepted idea of very short magnetic coherence lengths of a few interatomic spacings, or, equivalently, of the spin-transfer torques as an interface property[.5,](#page-4-6)[8,](#page-4-9)[11](#page-5-2)[,23](#page-5-14) Very recently, spin-transfer torques in antiferromagnetic metallic FeMn layers have been investigated theoretically;  $24$  it has been shown that the torques are not localized to the interface but are effective over the whole FeMn layer. However, no oscillatory behavior of the total torkance as a function of the layer thickness has been reported. The nature of the predicted oscillations deserves thus detailed analysis, including also a discussion of their stability with respect to structural imperfections and of their absence in the conductance [see Fig.  $2(a)$  $2(a)$ ].

Oscillations similar to those in Fig.  $2(a)$  $2(a)$  have recently been obtained for a different quantity of a simpler system, namely, for the spin-mixing conductance  $C<sup>mix</sup>$  of epitaxial fcc  $(001)$  Ni thin films attached to Cu leads.<sup>16</sup> The real and imaginary parts of the complex *C*mix are related to two components of the spin torque experienced by the FM film due to a spin accumulation in one of the NM leads; $5$  the calculated values of  $C^{\text{mix}}$  for the Cu/Ni/Cu(001) system are shown in Fig.  $2(b)$  $2(b)$ . The oscillation periods of the torkance and the spin-mixing conductance are identical which indicates a

<span id="page-3-1"></span>

FIG. 3. (Color online) Calculated in-plane  $(C_{\parallel})$  and out-of-plane  $(C_{\perp})$  Ni torkances (per interface atom) as functions of Ni thickness in spin valves Cu/Co/Cu/Ni/Cu(001) for  $\theta = \pi/2$ , 10 ML Cu spacer and for three different Co thicknesses.

common origin of both. The physical mechanism behind the *C*mix oscillations was identified with an interference effect between spin-↑ electrons propagating across the Ni film from the  $R$  lead to the  $L$  lead and spin- $\downarrow$  electrons propagating backward. This effect is expressed by a spin-mixing term  $\sim$ tr( $\Gamma_R G^r \Gamma_L G^q$ ) in the *C*<sup>mix</sup>, where the  $G^{r,\bar{q}}_s(s = \uparrow, \downarrow)$  denote spin-resolved propagators and the trace (tr) does not involve the spin index.<sup>16</sup> The particular value of the oscillation period follows from a special shape of the spin-polarized Fermi surface of bulk fcc Ni.<sup>16</sup>

The oscillations of *C*mix have been found fairly stable against Cu-Ni interdiffusion at the interfaces; $25$  the same stability can be thus expected for the torkance oscillations in the spin valve. The relative stability can be understood as an effect of the large oscillation period  $(\sim 12$  ML): intermixing confined to a very few atomic planes at interfaces reduces the oscillation amplitude rather weakly. This feature contrasts, e.g., sensitivity of the interlayer exchange coupling in magnetic multilayers mediated by a NM  $Cu(001)$  spacer with oscillation periods of  $\sim$ 2.5 and 6 ML, where even a very small amount of interface disorder reduces strongly especially the amplitude of the short-period oscillations.<sup>2</sup>

Another important aspect of the oscillations of the spintransfer torques concerns their dependence on the thickness of the polarizing Co layer since ultrathin layers in general might amplify ballistic and interference effects. Figure [3](#page-3-1) presents the Ni torkances in the same Cu/Co/Cu/Ni/Cu(001) spin valves calculated for three different Co thicknesses, namely, 5, 15, and 25 ML. It can be seen that the oscillations persist and have the same period in all three cases. Their amplitudes depend slightly on the Co thickness: the initial increase from 5 to 15 Co ML is accompanied by a small reduction (of about 20  $%$ ) in the amplitudes whereas further increase from 15 to 25 Co ML does not influence them appreciably. More detailed investigation of the effect of the thickness of the polarizing Co layer, including also the limiting case of spin valves FM1/NM/FM2/NM with a semiinfinite polarizing FM lead, $9$  is beyond the scope of the present study.

Let us now discuss the absence of oscillations in the con-ductance [Fig. [2](#page-3-0)(a)]. We introduce propagators  $G_2^{r,a}$  of an

auxiliary system NM/NM1/NM/FM2/NM, where NM1 denotes the FM1 layer with null exchange splitting. These propagators satisfy  $G^{r,a} = G_2^{r,a} + G_2^{r,a} T_1^{r,a} G_2^{r,a}$  where the  $T_1^{r,a}$  denotes the *t* matrix corresponding to the FM1 exchange splitting  $\gamma_1$  $\gamma_1$  in Eq. (1). The conductance Eq. ([13](#page-1-6)) can be then rewritten as  $C = (2\pi)^{-1} \text{Tr}(\Gamma_{\mathcal{R}} G_2^r \Delta_{\mathcal{L}} G_2^q)$ , where  $\Delta_{\mathcal{L}} = (1$  $+T_1^r G_2^r \Gamma_{\mathcal{L}}(1+G_2^a T_1^a)$  represents an operator localized at the FM1 layer, i.e., at the left end of the FM2 layer. The latter trace can be most easily evaluated using the spinquantization axis parallel to the FM2 magnetization direction  $\mathbf{n}_2$ . Since the propagators  $G_2^{r,a}$  are now diagonal in the spin index *s* and the operator  $\Gamma_{\mathcal{R}}$  is spin independent, the conductance does not contain spin-mixing terms, i.e., terms  $\sim$ tr( $\Gamma_{\mathcal{R}} G_{2,s}^r \Delta_{\mathcal{L},ss'} G_{2,s'}^a$ ) for  $s \neq s'$  that result in interference effects involving different spin channels. For the torkance, however, the extra factor  $\mathbf{n}_1 \cdot \boldsymbol{\sigma}$  in Eq. ([14](#page-1-5)) provides the necessary spin mixing responsible for the oscillations, in full analogy to oscillations of the spin-mixing conductance.

A recent study of spin-transfer torques in a tunnel junction Cu/Fe/MgO/Fe/Cu has predicted torkance and conductance oscillations with Fe thickness with a period  $\sim$  2 ML.<sup>8</sup> These oscillations were ascribed to quantum-well states in the majority spin of the Fe layer, i.e., to interference effects in a single spin channel. The oscillations in the Cu/Co/Cu/Ni/Cu system—manifested only in the torkance—have thus a clearly different origin.

#### **IV. CONCLUSION**

We have addressed two important aspects of spin-transfer torques in noncollinear spin valves with ultrathin layers. First, we have shown that the in-plane and out-of-plane torkance on one FM layer can be expressed by means of the transmission and reflection coefficients, respectively, of the whole spin valve, in close analogy to the Landauer formula for the ballistic conductance. Second, a novel oscillatory behavior for Ni-based systems has been predicted due to the mixed spin channels. The oscillations with Ni thickness are reasonably stable with respect to interface imperfections of real samples; however, they are not present in the conductance but can be observed only in the Ni torkance. The torkance oscillations prove that the spin-transfer torques in ballistic spin valves are closely related to properties of their components, in particular to the spin-mixing conductances of individual ferromagnetic layers.

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## **APPENDIX: PROOF OF THE COMMUTATION RULE FOR SELF-ENERGY**

The proof of the commutation rule Eq.  $(10)$  $(10)$  $(10)$  rests on assumed properties of the operators  $H$ ,  $Q$ , and  $D$  (defined in the Hilbert space of the total system) and of the projectors  $\Pi_{\mathcal{L}}$ ,  $\Pi_{\mathcal{R}}$ , and  $\Pi_{\mathcal{I}}$ , see the beginning of Sec. [II B.](#page-0-1) Let as abbreviate projections of any operator *X*  $(X=H, Q, D)$  as  $\Pi_X X \Pi_Z = X_{\mathcal{I} \mathcal{I}}$ ,  $\Pi$ <sub>*TX*</sub>**I**I<sub>*l*</sub> =  $X$ <sub>*Tl*</sub>, etc. The assumed property of *Q*, namely, *Q*  $=Q_{LL}+Q_{TT}+Q_{RR}$ , a consequence of the localization of *D* in *T*, namely,  $D_{\mathcal{IL}}=0$  and  $D_{\mathcal{LT}}=0$ , and the orthogonality of the projectors  $\Pi_{\mathcal{L}}$ ,  $\Pi_{\mathcal{R}}$ , and  $\Pi_{\mathcal{I}}$  lead to identities

$$
Q_{\mathcal{I}\mathcal{I}}H_{\mathcal{I}\mathcal{L}} = H_{\mathcal{I}\mathcal{L}}Q_{\mathcal{L}\mathcal{L}}, \quad Q_{\mathcal{L}\mathcal{L}}H_{\mathcal{L}\mathcal{I}} = H_{\mathcal{L}\mathcal{I}}Q_{\mathcal{I}\mathcal{I}}.
$$
 (A1)

<span id="page-4-11"></span><span id="page-4-10"></span>Similarly, a commutation rule

$$
Q_{\mathcal{L}\mathcal{L}}H_{\mathcal{L}\mathcal{L}} = H_{\mathcal{L}\mathcal{L}}Q_{\mathcal{L}\mathcal{L}}
$$
 (A2)

can easily be obtained from  $D_{LL}=0$ .

<span id="page-4-12"></span>The left self-energy is given explicitly by

$$
\Sigma_{\mathcal{L}}^{r,a}(E) = H_{\mathcal{IL}} \mathcal{G}_{\mathcal{L}}^{r,a}(E) H_{\mathcal{LI}},\tag{A3}
$$

where the  $\mathcal{G}_L^{r,a}(E)$  denotes the retarded and advanced propagator of the isolated left lead. The relation  $(A2)$  $(A2)$  $(A2)$  implies immediately a commutation rule

$$
Q_{\mathcal{L}\mathcal{L}}\mathcal{G}_{\mathcal{L}}^{r,a}(E) = \mathcal{G}_{\mathcal{L}}^{r,a}(E)Q_{\mathcal{L}\mathcal{L}};
$$
 (A4)

its application together with Eqs.  $(A1)$  $(A1)$  $(A1)$  and  $(A3)$  $(A3)$  $(A3)$  leads to identities

$$
Q_{\mathcal{I}\mathcal{I}}\Sigma_{\mathcal{L}}^{r,a}(E) = Q_{\mathcal{I}\mathcal{I}}H_{\mathcal{I}\mathcal{L}}\mathcal{G}_{\mathcal{L}}^{r,a}(E)H_{\mathcal{L}\mathcal{I}} = H_{\mathcal{I}\mathcal{L}}\mathcal{Q}_{\mathcal{L}\mathcal{L}}\mathcal{G}_{\mathcal{L}}^{r,a}(E)H_{\mathcal{L}\mathcal{I}}
$$
  
\n
$$
= H_{\mathcal{I}\mathcal{L}}\mathcal{G}_{\mathcal{L}}^{r,a}(E)\mathcal{Q}_{\mathcal{L}\mathcal{L}}H_{\mathcal{L}\mathcal{I}} = H_{\mathcal{I}\mathcal{L}}\mathcal{G}_{\mathcal{L}}^{r,a}(E)H_{\mathcal{L}\mathcal{I}}\mathcal{Q}_{\mathcal{I}\mathcal{I}}
$$
  
\n
$$
= \Sigma_{\mathcal{L}}^{r,a}(E)Q_{\mathcal{I}\mathcal{I}},
$$
 (A5)

which are equivalent to the commutation rule Eq.  $(10)$  $(10)$  $(10)$  for the left self-energy. The proof for the right self-energy is similar and therefore omitted.

<span id="page-4-0"></span>\*carva@karlov.mff.cuni.cz

- <span id="page-4-1"></span>† Also at Institute of Physics of Materials, Academy of Sciences of the Czech Republic, CZ-61662 Brno, Czech Republic; turek@ipm.cz
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