# **Free-electron model of current-induced spin-transfer torque in magnetic tunnel junctions**

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Spin and charge transport in a biased planar tunnel junction with two ferromagnetic electrodes are analyzed theoretically in the spin-polarized free-electron-like model. Tunneling current and both in-plane and out-ofplane components of the current-induced spin torque exerted on ferromagnetic components of the junction are determined as a function of the angle between magnetic moments of the electrodes, barrier height and thickness, and spin polarization of the electrodes. The out-of-plane component of the torque is found to be comparable in magnitude to the in-plane component. Numerical results for junctions with sufficiently high barriers show that the in-plane torque exerted on the sink electrode increases monotonically with increasing spin polarization (spin splitting) of the electron band in the source electrode, while the out-of-plane torque increases with increasing spin polarization of the electron bands in both electrodes. In junctions with thick and low barriers, the torque components can change their sign. The bias voltage dependence of the in-plane torque is not symmetric with respect to the bias reversal, even in symmetric junctions. When one of the ferromagnetic electrodes is replaced by a ferromagnetic layer of finite thickness (followed by a nonmagnetic electrode), both components of the spin torque depend significantly on the layer thickness due to the size effect and quantum well states formed in the thin magnetic layer.

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## **I. INTRODUCTION**

It is well known that electrical resistance of a tunnel junction consisting of two ferromagnetic electrodes and a nonmagnetic barrier depends on relative orientation of the electrodes' magnetic moments. Moreover, the resistance is usually larger when the magnetic moments are antialigned (antiparallel configuration) and smaller when the moments are oriented in the same direction (parallel configuration). This phenomenon is known as the tunnel magnetoresistance  $(TMR)$  effect<sup>1</sup> and is similar to the giant magnetoresistance (GMR) observed in system with a nonmagnetic metallic layer instead of the tunnel barrier.<sup>2</sup> Both TMR and GMR effects are suitable for applications, for instance, in nonvolatile magnetic random access memories, $3$  weak magnetic field sensors, and other spintronics devices.

Systems which exhibit the GMR or TMR effect also reveal another interesting phenomenon, i.e., the current induced magnetic switching (CIMS), whose physics is closely related to that responsible for GMR and TMR. The CIMS phenomenon is a consequence of an additional torque exerted on film's magnetization, which in turn is a result of spin transfer from conduction electrons to localized magnetic moments. The presence of such a spin torque in metallic structures consisting of two magnetic layers separated by a nonmagnetic spacer with noncollinear alignment of the layers' magnetic moments has been predicted theoretically by Slonczewski<sup>4</sup> and Berger.<sup>5</sup> Similar phenomenon also has been predicted for magnetic tunnel junctions. $1,6$  $1,6$  In all cases, the current-induced magnetic switching occurs for the current density exceeding a certain critical value.

In the systems discussed above, electric current (more precisely, the associated spin current) usually destabilizes one of the two collinear magnetic configurations and stabilizes the other one. As a result, current can induce transition either from the parallel to antiparallel configurations or vice versa. When, for instance, the current flowing in a certain direction leads to the parallel to antiparallel transition, the current flowing in the opposite direction usually restores the parallel orientation. In some systems, however, current can destabilize both parallel and antiparallel configurations for one bias polarization and stabilize both configurations for the opposite bias. In such unconventional systems, the current can induce transition to the processional regime, where magnetic moment of a ferromagnetic (sensing) film rotates with the frequency in the microwave range without any magnetic field.<sup> $\frac{7}{1}$ </sup> The transition to precessional regime is also possible in systems with conventional CIMS phenomena when an external magnetic field is applied.

The current-induced switching of a magnetic moment was studied experimentally first in metallic nanopillars.<sup>8[,9](#page-8-9)</sup> In typical systems such as Co/Cu/Co spin valves, the critical current is of the order of  $10^7$  A/cm<sup>2</sup>.<sup>[9](#page-8-9)</sup> Due to a relatively high critical current density required for magnetic switching, the systems including tunnel barriers (where the current flowing due to the quantum-mechanical tunneling effect is usually smaller) got not so much attention as the metallic structures. However, it has been demonstrated experimentally that CIMS can be also observed in tunnel junctions $10-13$  for a sufficiently large current density. For instance, the critical current needed to change magnetic configuration of a tunnel junction including ferromagnetic layers of CoFeB separated by a nonmagnetic barrier of MgO is of the order of 10<sup>6</sup> A/cm2 . [12](#page-8-12) These observations stimulated further experimental and theoretical works aimed at understanding physical mechanism of the CIMS phenomenon in magnetic tunnel iunctions. $14-16$ 

In a recent paper, Theodonis *et al.*[14](#page-8-13) found that the two, in-plane and out-of-plane (normal), components of the spin torque in tunnel junctions are of comparable magnitude. They considered a tunnel junction consisting of two semiinfinite ferromagnetic electrodes separated by a nonmagnetic barrier and calculated the spin torque using the Green's function technique. They also found an anomalous variation of the spin torque with the bias voltage. Here, we calculate the spin torque by a different method and also go beyond the approximation of semi-infinite electrodes by considering the situation with one ferromagnetic electrode replaced by a thin ferromagnetic layer followed by a nonmagnetic semiinfinite electrode). Such a structure is interesting for two reasons. (i) In typical experimental systems one magnetic layer is relatively thick, while the second one (sensing layer) is very thin. (ii) Finite thickness of the sensing layer has a significant influence on the tunneling current and spin torque due to the size effect and quantum well states formed in this layer. We calculate the spin torque induced by a charge current (more precisely, the torque due to a spin current associ-ated with the charge current). We do not take into account the "conservative" torque which appears in equilibrium situation as an exchange coupling between the ferromagnetic electrodes.

Both the in-plane and out-of-plane components of the spin torque exerted on the two magnetic components of the junction are calculated and analyzed as a function of the angle between magnetic moments, spin splitting of the electron bands in electrodes, height and thickness of the barrier, and also thickness of the thin magnetic layer. It is shown that the in-plane component of the spin torque exerted on a particular ferromagnetic electrode (film) is not symmetric with respect to the bias reversal, even in junctions with both identical electrodes, which is in agreement with the results obtained in Ref. [14.](#page-8-13) Apart from this, the sign of spin torque component can oscillate with thickness of the thin sensing layer.

The paper is organized as follows. First, in Sec. II, we describe the model and present general formulae for the spin current and spin torque. Numerical results are presented and discussed in Sec. III. Summary and final conclusions are in Sec. IV.

### **II. MODEL AND BASIC THEORETICAL FORMULAS**

We consider a tunnel junction consisting of two ferromagnetic layers separated by a nonmagnetic barrier, as shown schematically in Fig. [1.](#page-1-0) One of the ferromagnetic layers (the left one) is assumed to be thick enough to be considered as semi-infinite and playing the role of left electrode. Its magnetic moment is assumed to be fixed in the junction plane. The second magnetic layer (the right one) is of arbitrary thickness and its magnetic moment is free to rotate under the influence of external magnetic field or electric current. When this layer is sufficiently thick, it may be treated as a (semiinfinite) right electrode. If, however, it is relatively thin, then we assume that it is followed by a thick (semi-infinite) nonmagnetic layer considered as the right electrode.

Two local coordinate systems (one for each ferromagnetic layer) are introduced to describe spin polarization of the tunneling electrons. The axis  $z(z')$  of the local system in the left (right) magnetic layer is oriented along the corresponding net spin moment. To describe the electron spin in the barrier, we use the local coordinate system of the left ferromagnetic

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

FIG. 1. Schematic picture of a single planar tunnel junction. *S<sup>l</sup>* and *S<sup>r</sup>* represent the spin moments of the two ferromagnetic layers, while  $T_{\parallel}$  and  $T_{\perp}$  are the two components of the spin torque exerted on the right magnetic layer. The local coordinate systems introduced for both layers are also shown.

electrode. Furthermore, we assume that the axes  $x$  and  $x'$  are in the plane formed by the two magnetic moments. The axes *y* and *y* coincide then and are perpendicular to this plane. When magnetic moments of the ferromagnetic films are in the corresponding layer planes, the axes  $y$  and  $y'$  are also perpendicular to the magnetic films, as shown in Fig. [1.](#page-1-0) Since the torque depends only on the angle  $\theta$  between magnetic moments, independently on whether they are in the film plane or not, the following description will be restricted, without loss of generality, to the situation shown in Fig. [1,](#page-1-0) i.e., to the case of in-plane magnetic moments.

In this paper, we calculate the current-induced spin torque exerted on both ferromagnetic layers. The torque is normal to the corresponding spin moment, and we calculate both its components. One component, called the in-plane torque, is oriented in the plane formed by both magnetic moments and is oriented along the axis  $x(x')$  for the left (right) film. The second component, called the out-of-plane (or normal) torque, is perpendicular to the plane formed by the magnetic moments and is along the axis  $y(y'=y)$ .

We will use the definition according to which the charge current is positive when it flows from the thin (sensing) magnetic layer toward the thick one. Thus, for positive bias voltage, the electrons (and associated spin momentum) flow from the left to the right electrode. The two components of spin torque exerted on the ferromagnetic films are then determined from the appropriate components of the spin current. Accordingly, the in-plane and out-of-plane components of the spin torque exerted per unit square of the left ferromagnetic electrode can be calculated from the formulas<sup>17</sup>

and

$$
T'_{\parallel} = -\frac{\hbar}{2} J_x^{sl} \tag{1}
$$

$$
T_{\perp}^{l} = -\frac{\hbar}{2} J_{y}^{sl},\tag{2}
$$

respectively, where  $J^{\text{sl}}_{\mu}$  denotes the  $\mu$ th component  $(\mu = x, y)$ of the spin current density calculated in the barrier at a point located near the interface with the left electrode. Since all components of the spin current are independent of the position in the barrier, they can be taken at an arbitrary point inside the barrier.

<span id="page-2-0"></span>The torque exerted on the sensing (right) magnetic layer can be calculated in a similar way (taking into account the fact that the axes  $y$  and  $y'$  are equivalent),

$$
T_{\parallel}^r = \frac{\hbar}{2} \left[ J_{x'}^{sr} - \tilde{J}_{x'}^{sr} \right],\tag{3}
$$

$$
T'_{\perp} = \frac{\hbar}{2} [J_y^{sr} - \tilde{J}_y^{sr}], \tag{4}
$$

<span id="page-2-1"></span>where  $J_{x'}^{sr}$  and  $J_{y}^{sr}$  are the  $x'$  and y components of the spin current density, calculated in the barrier at a point close to the interface with the right ferromagnetic layer (practically, the spin currents can be taken anywhere in the barrier). In turn,  $\tilde{J}^{sr}_{x'}$  and  $\tilde{J}^{sr}_{y}$  denote the *x'* and *y* components of the spin current density calculated in a point located in the right nonmagnetic electrode close to the interface with the right ferromagnetic layer. These components represent the part of spin current density that is not absorbed in the ferromagnetic layer, but transmitted further to the right nonmagnetic electrode. When the right ferromagnetic layer is sufficiently thick (or semi-infinite), the  $x'$  and  $y$  components of the spin current perpendicular to the corresponding magnetization are totally absorbed by the layer and the terms  $\tilde{J}^{sr}_{x'}$  and  $\tilde{J}^{sr}_{y}$  in Eqs. ([3](#page-2-0)) and ([4](#page-2-1)) vanish exactly. In such junctions, the magnitudes of the out-of-plane torques exerted on both ferromagnetic layers are the same.

The spin current densities  $J_{x}^{sr}$  and  $\tilde{J}_{x'}^{sr}$  are written in the local coordinate system of the right ferromagnetic layer. They can be transformed to the coordinate system of the left magnetic layer as

$$
J_{x'}^{sr} = J_x^{sr} \cos \theta + J_z^{sr} \sin \theta, \tag{5}
$$

where  $J_z^{sr}$   $(J_x^{sr})$  is the  $z(x)$  component of the spin current density in the barrier. Similar rotation formula also holds for  $\widetilde{J}^{sr}_{x'}$ .

To find the spin torque, one needs first to determine the relevant spin current components. Generally, the  $\mu$ th component  $(\mu = x, y, z \text{ or } \mu = x', y', z')$  of the spin current density  $j^s_\mu(y)$  corresponding to electrons described by the wave function  $\Psi(y)$  is given by

<span id="page-2-2"></span>
$$
j_{\mu}^{s}(y) = \frac{i\hbar}{2m} \left[ \left( \frac{\partial}{\partial y} \Psi^{+}(y) \right) \sigma_{\mu} \Psi(y) - \Psi^{+}(y) \sigma_{\mu} \frac{\partial}{\partial y} \Psi(y) \right],
$$
\n(6)

where  $\sigma_{\mu}$  are the Pauli matrices, and the electron wave function  $\Psi(y)$  has the spinor form,

$$
\Psi = \begin{bmatrix} \psi_{\uparrow}(y) \\ \psi_{\downarrow}(y) \end{bmatrix},
$$

with  $\psi_{\uparrow}(y)$  and  $\psi_{\downarrow}(y)$  being the two spinor components in the relevant local reference frame. From the general expression [Eq. ([6](#page-2-2))], one can easily find the formula for all components of the spin current density. In particular, the *z* component can be calculated as

$$
j_z^s(y) = \frac{\hbar}{m} \operatorname{Im} \sum_{\sigma} \hat{\sigma} \psi_{\sigma}^* \left[ \frac{d\psi_{\sigma}}{dy} \right],
$$
 (7)

<span id="page-2-3"></span>where  $\hat{\sigma}$ =1 when  $\sigma$ = $\uparrow$  and  $\hat{\sigma}$ = $-1$  for  $\sigma$ = $\downarrow$ . The other components of the spin current can be calculated from the formula[s1](#page-8-1)

$$
j_x^s(y) = \text{Re } j_+^s(y)
$$
 (8a)

and

$$
j_y^s(y) = \text{Im } j_+^s(y),
$$
 (8b)

where  $j^s_+(y)$  is defined as

$$
j_{+}^{s}(y) = \frac{i\hbar}{m} \left[ \frac{d\psi_{\uparrow}^{*}}{dy} \psi_{\downarrow} - \psi_{\uparrow}^{*} \frac{d\psi_{\downarrow}}{dy} \right].
$$
 (9)

<span id="page-2-5"></span>The charge current density, in turn, is given by

$$
j(y) = \frac{e\hbar}{m} \operatorname{Im} \sum_{\sigma} \psi_{\sigma}^* \left[ \frac{d\psi_{\sigma}}{dy} \right].
$$
 (10)

In this paper, we assume the free-electron-like model, with the electronic structure of ferromagnetic and nonmagnetic layers modeled by a parabolic band of free electrons. This band is spin split in the case of ferromagnetic layers. The wave function of an electron with spin  $\sigma$ , propagating in the *i*th layer  $(i=l$  and  $i=r$  for the left and right magnetic films, respectively, and  $i = r'$  for the right nonmagnetic electrode) along the direction normal to the layer, takes the standard form

$$
\psi_{i\sigma} = A_{i\sigma} \exp(ik_{i\sigma}y) + B_{i\sigma} \exp(-ik_{i\sigma}y), \qquad (11)
$$

where  $k_{i\sigma}$  is the perpendicular (to the layer) component of the electron wave vector in the *i*th layer and  $A_{i\sigma}(B_{i\sigma})$  are the relevant amplitudes. When electrons with spin  $\sigma$  are incident on the barrier from the left, we set  $A_{l\sigma} = 1$  and  $A_{l\bar{\sigma}} = 0$  (where  $\overline{\sigma} = -\sigma$ ). For the right electrode, we set  $B_{r\sigma} = 0$  (or  $B_{r'\sigma} = 0$  in the case of a thin right magnetic layer) for both values of  $\sigma$ (there is no reflected waves in the right electrode). For electrons of the total energy  $E$ ,  $k_{i\sigma}$  can be determined from the formula

$$
k_{i\sigma} = \sqrt{\frac{2m(E - E_{i\sigma}^b)}{\hbar^2} - k_{\parallel}^2} = \frac{\sqrt{2m(\varepsilon_{\perp} - E_{i\sigma}^b)}}{\hbar},\qquad(12)
$$

where  $E_{i\sigma}^{b}$  denotes the electron band bottom for spin  $\sigma$  in the *i*th layer,  $k_{\parallel}$  is the in-plane component of the wave vector,  $\varepsilon_{\perp} = E - \hbar^2 k_{\parallel}^2 / 2m$  is the electron energy associated with its motion in the direction perpendicular to the layers, and *m* is the free electron mass.

In turn, the wave function corresponding to electrons propagating in the barrier along the axis *y* has the form

$$
\psi_{\sigma B} = C_{B\sigma} \text{Ai}(Z) + D_{B\sigma} \text{Bi}(Z),\tag{13}
$$

<span id="page-2-4"></span>where  $Ai(Z)$  and  $Bi(Z)$  are the Airy functions, and the argument *Z* is a function of *y*,

$$
Z(y) = \left(\frac{d\sqrt{2m}}{\hbar eV}\right)^{2/3} \left(U - eV\frac{\Delta y}{d} - \varepsilon_{\perp}\right),\tag{14}
$$

with *V* denoting the bias voltage applied to the junction, *U* and *d* representing the barrier height and barrier thickness, respectively, and  $\Delta y$  standing for the distance of the point *y* in the barrier from the interface with the source electrode.

The constants  $A_{i\sigma}$ ,  $B_{i\sigma}$ ,  $C_{B\sigma}$ , and  $D_{B\sigma}$  in Eqs. ([11](#page-2-3)) and ([13](#page-2-4)) (generally different in different layers) can be determined from the continuity conditions of the electron wave function and its first derivative at the interfaces between different layers. In the case of the interface between barrier and right ferromagnetic layer, the change in the quantization axis requires spinor transformation, so the wave function continuity conditions read<sup>1</sup>

$$
\psi_{\uparrow B} = \psi_{\uparrow r} \cos\left(\frac{\theta}{2}\right) + \psi_{\downarrow r} \sin\left(\frac{\theta}{2}\right),\tag{15a}
$$

$$
\psi_{\downarrow B} = -\psi_{\uparrow r} \sin\left(\frac{\theta}{2}\right) + \psi_{\downarrow r} \cos\left(\frac{\theta}{2}\right). \tag{15b}
$$

To calculate the components of the total spin current density, one needs to sum up contributions from electrons of different total energy and in-plane wave vector components. In the zero temperature limit, the charge and spin currents are determined by electrons from the energy window between the Fermi levels in the sink and source electrodes. Taking this into account and assuming the left (right) electrode as the source (drain), one can write the  $\mu$ th component of bias-induced spin current density in the form

$$
J_{\mu}^{s}(y) = \frac{4\pi^{2}m^{2}}{h^{4}} \sum_{\sigma} \left[ \int_{E_{l\sigma}^{b}}^{E_{F}-eV} d\varepsilon_{\perp} \frac{eV}{k_{l\sigma}(\varepsilon_{\perp})} j_{\mu}^{s}(y, \varepsilon_{\perp}) + \int_{E_{F}-eV}^{E_{F}} d\varepsilon_{\perp} \frac{(E_{F}-\varepsilon_{\perp})}{k_{l\sigma}(\varepsilon_{\perp})} j_{\mu}^{s}(y, \varepsilon_{\perp}) \right],
$$
 (16)

where  $E_F$  is the Fermi energy in the source electrode, and the dependence of  $k_{l\sigma}$  and  $j^s_{\mu}$  on  $\varepsilon_{\perp}$  is explicitly written. The integration is performed over the energy associated with the motion perpendicular to the layer planes, whereas the summation is over the two spin subbands. The total charge current can be calculated from a similar formula, with  $j^s_\mu$  replaced by  $j$  calculated from Eq.  $(10)$  $(10)$  $(10)$ .

From our calculations also follows that the in-plane spin torque in junctions with both semi-infinite electrodes can be related to the spin currents flowing in the parallel and antiparallel configurations and carried by electrons of both spin orientations. The relevant formula, which connects the spin torque to the above mentioned currents, was proposed in Ref. [14.](#page-8-13) We have checked numerically the correctness of Eq.  $(6)$ from Ref. [14](#page-8-13) and found that the results for in-plane torque in systems with semi-infinite electrodes, calculated on the basis of this formula, roughly coincide with those presented in our paper. This results from the fact that the in-plane component of the torque can be expressed in terms of the four charge currents, as pointed out by Slonczewski.<sup>6</sup> These currents can be approximated by the currents flowing in the parallel and antiparallel configurations and carried by spin-up and spin-

down electrons, which leads to formula (6) in Ref. [14.](#page-8-13) This approximation is well justified for junctions with high and thick barriers, but leads to reasonable results also in junctions with barriers of height and thickness studied practically in all experiments (as well as in our paper).

### **III. NUMERICAL RESULTS**

Numerical calculations have been performed for both semiconductor and metallic junctions. It turned out that the results do not depend significantly on the junction type, provided the ratio of the barrier height and average electron band width as well as the spin polarization of the ferromagnetic films are kept constant. Therefore, we limit the following discussion to the junctions with metallic electrodes. According to Ref. [18,](#page-8-16) a dominant contribution to the tunneling current in junctions composed of Fe electrodes and  $Al_2O_3$ barriers is given by electrons from the spin-split parabolic band, which can be well described by the Fermi energy  $E_F$ = 2.62 eV and half of the spin splitting  $\Delta = \Delta_i = \Delta_i = 1.96$  eV (with  $\Delta_l$  and  $\Delta_r$  denoting half of the spin splitting in the left and right ferromagnetic films, respectively). The barrier height, measured from the Fermi level in the source electrode, is commonly assumed to be equal to  $U=1.5$  eV in such junctions, whereas the barrier thickness can be taken as  $d = 0.7$  nm. Optimal  $Al_2O_3$  barrier thickness needed to obtain large magnetoresistance varies from  $0.7$  to  $1.8$  nm, <sup>19</sup> although a nonvanishing TMR was also found in systems with  $d = 0.4$  nm.<sup>[19](#page-8-17)</sup> Our calculations have been performed for a relatively thin barrier  $(d=0.7 \text{ nm})$ , which allows us to obtain high charge and spin current densities, and consequently, also a large spin torque.

# **A. Torque in symmetric junctions with both semi-infinite electrodes**

We begin with the junctions whose both magnetic films are sufficiently thick to be considered as semi-infinite electrodes, but thin enough to justify application of the ballistic description. Such a description is valid either if the electrode is thin compared to the corresponding mean free path, or if the transverse spin current is fully absorbed by the electrode within the mean free path. The situation with one magnetic film being thin enough to reveal size effects will be considered later.

The out-of-plane  $(y)$  and in-plane  $(x')$  components of the spin-transfer torque exerted on the right ferromagnetic electrode as well as the charge current flowing along the axis  $-y$ ), calculated as a function of the angle  $\theta$  between magnetic moments of the leads, are presented in Fig. [2](#page-4-0) for the bias voltage  $V= 0.5$  V. The charge current density is shown for  $\Delta = 1.96$  eV [see Fig. [2](#page-4-0)(c)], whereas spin torque in Figs. 2(a) and  $2(b)$  $2(b)$  is shown for three different values of  $\Delta$ . Both components of the torque are of comparable magnitude, $14$  though the in-plane component is slightly larger than the normal one. This is in contrast to the results obtained for metallic spin valve nanopillars, where the normal component is negligibly small in comparison to the in-plane one.<sup>17</sup> In the tunnel junctions considered here, the magnitude of both compo-

<span id="page-4-0"></span>

FIG. 2. The (a) out-of-plane and (b) in-plane components of the spin torque exerted on the right ferromagnetic electrode as well as (c) the corresponding charge current density calculated as a function of  $\theta/\pi$ . The parameters assumed for the junction are the Fermi energy  $E_F$ = 2.62 eV, barrier height  $U$ = 1.5 eV, barrier thickness *d*  $= 0.7$  nm, and the bias voltage  $V = 0.5$  V. The different lines correspond to different values of the spin splitting of electron bands in the electrodes.

nents increases with increasing spin polarization of the ferromagnetic electrodes (increasing  $\Delta$ ). As one might expect, the torque vanishes in the collinear configurations and achieves a maximum absolute value for  $\theta = \pi/2$  (and  $\theta$ )  $= 3\pi/2$ , i.e., when magnetic moments of the electrodes are oriented perpendicularly. For positive bias assumed in Fig. [2](#page-4-0) (electrons flow from left to the right), the torque stabilizes parallel configuration and destabilizes antiparallel one. In turn, the charge current is maximal in the parallel configuration and decreases monotonically when magnetic moments rotate toward the antiparallel configuration. Therefore, when plotting the normalized torque (torque divided by the charge current), the corresponding maxima are shifted to  $\theta > \pi/2$ and  $\theta < 3\pi/2$ , respectively.

Further calculations show that the results presented in Fig. [2](#page-4-0) do not change qualitatively as the width or height of the barrier is varied in junction with relatively high barriers. Especially, both torque components have maxima at the same values of  $\theta$  and have the same signs as in Fig. [2.](#page-4-0) However, the magnitude of the components decreases exponentially with increasing barrier width and this decrease is faster than that of the charge current. As a result, the normalized torque components decrease with increasing barrier width, as shown in Fig. [3](#page-4-1)(a) for  $\theta = \pi/2$ . A different behavior is found for the

<span id="page-4-1"></span>

FIG. 3. The normalized out-of-plane (dashed line) and in-plane (solid line) components of the spin torque exerted on the right ferromagnetic electrode, calculated as a function of the (a) barrier thickness and (b) barrier height for the angle  $\theta = \pi/2$ . The other parameters are the same as in Fig. [2.](#page-4-0)

dependence on the barrier height *U*. Now, the magnitude of both normalized torque components increases with increasing  $U$  [see Fig. [3](#page-4-1)(b)], which is a consequence of the fast decay of charge current.

A very peculiar situation occurs in junctions with considerably low and wide barriers. As shown in Fig. [4,](#page-5-0) for *U* = 0.6 eV and  $d = 1.0$  nm, the torque for  $\Delta = 0.98$  eV has then a sign opposite to that found previously for a high and thin barrier  $(U=1.5 \text{ eV}, d=0.7 \text{ nm})$ . Similar situation occurs in the case of in-plane torque for  $\Delta = 1.96$  eV; however, the torque magnitude is then smaller. The inversion of the torque sign results here from the inversion of the sign of the effective polarization of the tunneling electrons in junctions with a very low barrier. The effective polarization, introduced by Slonczewski, $<sup>1</sup>$  depends on the wave vectors corresponding to</sup> electrons of a specific spin orientation in ferromagnetic electrodes, as well as on the barrier height. In junctions with negative effective polarization, electrons with minority spin tunnel easier through the barrier and give dominant contribution to the tunneling current. Inversion of the effective polarization can also lead to an increase in TMR with bias voltage and to inverse TMR in asymmetric junctions. $1,19,20$  $1,19,20$  $1,19,20$ 

Now, we analyze the bias dependence of the spin torque exerted on the right ferromagnetic electrode. The results obtained for the out-of-plane and in-plane components in junctions with perpendicular magnetic moments  $(\theta = \pi/2)$  are presented in Fig. [5](#page-5-1) and are in qualitative and quantitative agreement with those of Ref. [14.](#page-8-13) The different lines corre-

<span id="page-5-0"></span>

FIG. 4. The (a) out-of-plane and (b) in-plane components of the torque exerted on the right ferromagnetic electrode and (c) the charge current density, calculated as a function of  $\theta/\pi$ . The parameters of the junction are the Fermi energy  $E_F = 2.62$  eV, barrier height  $U=0.6$  eV, barrier thickness  $d=1.0$  nm, and the bias voltage *V*= 0.5 V. The different lines correspond to different spin splitting of the electron bands in the electrodes.

spond to different spin splitting of the electron bands in the electrodes. The charge current density plotted for positive voltages is also given [the inset in Fig.  $5(b)$  $5(b)$ ]. The out-ofplane component of the spin torque in symmetric junctions is symmetric with respect to the bias reversal and reveals a parabolic-like dependence on the bias. On the other hand, the in-plane component is clearly asymmetric. The torque exerted on the right electrode is significantly larger for positive bias (the electrode is a sink) than for negative bias (when it is the source electrode), especially in systems with strong spin splitting of the electron bands. This can be explained as follows: The normalized in-plane component of the torque acting on the sink (source) electrode depends mainly on the effective polarization of tunneling electrons in the source (sink) electrode.<sup>6</sup> After applying a bias voltage to the junction, polarization of the sink electrode decreases, whereas polarization of the source electrode remains constant. This results in a significant decrease of the normalized torque acting on the source electrode, but such a decrease is not observed for the sink electrode. In the present system, the right electrode corresponds to the sink electrode for positive bias voltage and to the source electrode for negative bias, which finally leads to the asymmetry displayed in Fig. [5.](#page-5-1) The asymmetry is much more pronounced for the normalized torque. As can be seen in Fig.  $5(d)$  $5(d)$ , the in-plane torque exerted on

<span id="page-5-1"></span>

FIG. 5. Bias dependence of the (a) out-of-plane and (b) in-plane components of the torque exerted on the right electrode in a symmetric junction for  $\theta = \pi/2$ . The corresponding normalized torque components are shown in parts (c) and (d) for the out-of-plane and in-plane components, respectively. The other parameters of the junction are the same as in Fig. [2.](#page-4-0) Different lines correspond to different spin splittings of the electron bands in ferromagnetic electrodes. The inset in Fig.  $5(b)$  $5(b)$  shows the charge current density.

the sink electrode at first increases with increasing bias voltage, and then reaches a plateau, whereas the torque exerted on the source electrode decreases monotonically and even changes sign. The sign change of the in-plane torque for negative bias voltages can be related to the decrease of effective barrier height (leading to the sign change of the effective spin polarization). In systems with smaller  $\Delta$ , the sign change of the in-plane torque appears for lower bias voltages than in systems with larger  $\Delta$ . This is in agreement with the fact that the in-plane torque in systems with smaller  $\Delta$ changes sign from positive to negative for relatively higher barriers.

Additional calculations show that in systems with magnetic moments close to parallel configuration (small  $\theta$ ), the saturation of the in-plane torque for positive bias is less pronounced. It is also worth noting that in certain situations ( $\theta$ close to  $\pi$ , large  $\Delta$ ), the normalized in-plane torque can also decrease with the increasing positive bias voltage. The bias dependence of the normalized out-of-plane torque  $[Fig. 5(c)]$  $[Fig. 5(c)]$  $[Fig. 5(c)]$ is not very pronounced—its magnitude first increases, and then decreases at higher voltages.

<span id="page-6-0"></span>

FIG. 6. Bias dependence of the  $[(a)$  and  $(c)]$  in-plane and  $[(b)$ and (d)] out-of-plane components of the spin torque exerted on the right electrode in an asymmetric junction with different spin splittings of the electron bands in the left  $(2\Delta_l)$  and right  $(2\Delta_r)$  electrodes, calculated for  $\theta = \pi/2$ . The other parameters of the junction are the same as in Fig. [2.](#page-4-0) Different lines correspond to different spin-splitting of the electron bands in the  $[(a)$  and  $(b)]$  right or  $[(c)$ and (d)] left electrodes.

# **B. Torque in nonsymmetric junctions with both semi-infinite electrodes**

Consider now the spin torque in nonsymmetric junctions, with the ferromagnetic electrodes made from metals with different spin polarizations (described by  $\Delta_l$  and  $\Delta_r$ ). The appropriate bias dependence is shown in Fig. [6.](#page-6-0) The results clearly show [see Figs.  $6(a)$  $6(a)$  and  $6(c)$ ] that the in-plane component of the torque acting on a given electrode does not change significantly with its polarization, but strongly depends on the polarization of the second ferromagnetic electrode.

Different results are obtained for the out-of-plane torque component. Now, the splitting of electron band in both electrodes has a similar influence and the magnitude of the torque exerted on the source and sink electrodes is the same, even in junctions with different electrodes [results obtained for positive bias in Fig.  $6(b)$  $6(b)$  are the same as the ones shown in Fig.  $6(d)$  $6(d)$  for negative voltages]. Due to the different spin splittings of electron bands in both electrodes, the out-ofplane component of the spin torque in junctions with  $\Delta_l$  $\neq \Delta_r$  is not symmetric with respect to the bias reversal, al-

<span id="page-6-1"></span>

FIG. 7. Bias dependence of the normalized  $[(a)$  and  $(d)]$  in-plane and [(b) and (e)] out-of-plane components of the torque exerted on the right electrode, and  $[(c)$  and  $(f)]$  the charge current density in an asymmetric junction with different spin splittings of the electron band in left  $(2\Delta_l)$  and right  $(2\Delta_r)$  electrodes, calculated for  $\theta$  $=\pi/2$ . The other parameters of the junction are the same as in Fig. [2.](#page-4-0) Different lines correspond to different spin splittings of the electron bands in the  $[(a)-(c)]$  right and  $[(d)-(f)]$  left electrodes.

though the asymmetry is less pronounced than that obtained for the in-plane component.

Similar conclusions can be drawn for the normalized torques. The in-plane component of the torque acting on the right electrode is almost insensitive to the changes in  $\Delta_r$ , but strongly varies with  $\Delta_l$  [Figs. [7](#page-6-1)(a) and 7(d)]. This statement is in agreement with the prediction of Slonczewski, who analyzed the zero-bias in-plane torque in similar systems with the use of Bardeen's transfer Hamiltonian method.<sup>6</sup> A smaller, but still visible asymmetry appears in the bias dependence of the normalized out-of-plane torque [Figs.  $7(b)$  $7(b)$ and  $7(e)$  $7(e)$ ]. This asymmetry is additionally enhanced by the bias asymmetry of the charge current, which can be easily deduced from the *I*-*V* characteristics presented in Figs. [7](#page-6-1)(c) and  $7(f)$  $7(f)$  for different values of  $\Delta_r$  and  $\Delta_l$ , respectively.

### **C. Torque in junctions with one ferromagnetic layer of finite thickness**

Consider now the junction in which the right magnetic film is of finite thickness  $d_f$  and is followed by a nonmag-

<span id="page-7-0"></span>

FIG. 8. (a) The normal and (b) the in-plane spin torque exerting on the right ferromagnetic layer (solid line) and left ferromagnetic electrode (dotted line) as well as (c) the charge current density, calculated as a function of the thickness of the right ferromagnetic layer. The parameters of the ferromagnetic components of the junction and the tunneling barrier are the same as in Fig. [2.](#page-4-0) The position of the Fermi level in the right nonmagnetic electrode is the same as in the right ferromagnetic layer. The bottom of the electron band in right nonmagnetic electrode lies in the middle point between the bottoms of the spin-split electron subbands in the right ferromagnetic layer.

netic semi-infinite electrode. Such a layer usually plays a role of a quantum well for electrons of one spin direction and a step for electrons of opposite spin. As a result, quantum interference leads to oscillations of the charge current in each spin channel separately. The oscillations periods are determined mainly by the wavelength of electrons from the Fermi level in the source electrode, which tunnel normally through the barrier. Accordingly, these oscillation periods are approximately equal to half of the wavelength of those electrons in the magnetic layer and can be calculated from the expression  $d_{\sigma} = \lambda_{\sigma}/2 = \pi/k_{\sigma} = \pi\hbar/\sqrt{2m(E_f + \hat{\sigma}\Delta + eV)}$ , where  $\hat{\sigma}$ =1 for spin-up and  $\hat{\sigma}$ =−1 for spin-down electrons,  $\Delta$  denotes half of the spin-splitting of the electron band in the magnetic layer, and *V* is the bias voltage applied to the system. The periods for  $V=0.5$  V, estimated according to this formula, are equal to  $d_1 = 0.27$  nm and  $d_1 = 0.57$  nm and are in agreement with the results of numerical calculations. Superposition of the oscillations in the two spin channels leads to a very complex dependence of the charge and spin cur-

<span id="page-7-1"></span>

FIG. 9. Bias dependence of  $[(a)$  and  $(c)]$  the normal and  $[(b)$  and (d)] the in-plane normalized spin torque exerted on  $[(a)$  and  $(b)]$  the right ferromagnetic layer of thickness  $d_f = 1.0$  nm and  $[(c)$  and  $(d)]$ the left infinite electrode obtained for  $\theta = \pi/2$  (solid line) and  $\theta$  $=\pi/4$  (dotted line). The other parameters of the junction are the same as in Fig. [2.](#page-4-0)

rents (and consequently the spin torque) on the thickness  $d_f$ , as displayed in Fig. [8,](#page-7-0) for  $\theta = \pi/2$  and  $V = 0.5$  V. The spin torque acting on the right layer of finite thickness, as well as the one acting on the left electrode, depends on  $d_f$  in an oscillatory way. The amplitude of the oscillations decreases with increasing layer thickness  $d_f$ . In spite of the complex behavior of the presented functions, one can note that the average value of spin torque is roughly the same as in junction with two infinite ferromagnetic electrodes. Similar statement is true for the charge current.

The junctions with ferromagnetic electrode of the finite thickness are of particular interest as the magnetic moment of the thin magnetic layer can be easily rotated by external magnetic field and especially by a current flowing through the system. When current density exceeds some critical value, one can observe current-induced spin switching either to parallel or to antiparallel magnetic configuration.

Components of spin torque depend nonmonotonically on the bias voltage, and form of this dependence strongly changes with the thickness of the ferromagnetic layer. The bias voltage leads to a change in the position of the band bottom for electrons of both spin directions in the magnetic layer of finite thickness, and consequently, to the change in the position of resonance states, which strongly affects the

charge and spin currents. This leads to the nonmonotonous dependence of the normalized spin torque on the bias voltage. The bias dependence of the normalized torque acting on the right layer and on the left electrode is shown in Fig. [9](#page-7-1) [Figs.  $9(a) - 9(d)$  $9(a) - 9(d)$ , respectively] for the junction with  $d_f$ = 1.0 nm. Quasioscillations of the in-plane torque exerted on the source electrode can be seen in Fig.  $9(d)$  $9(d)$ . In general, magnitude of the torque is larger in junctions with perpendicular magnetic moments.

### **IV. SUMMARY**

We have calculated spin-transfer torque in ferromagnetic tunnel junctions. The numerical results have been obtained within the free-electron-like model of spin polarized electrons. We have considered numerically two different situations: (i) both magnetic films were sufficiently thick to be treated as semi-infinite ferromagnetic electrodes, and (ii) the left ferromagnetic film was thick, while the right one was thin and was followed then by a nonmagnetic electrode. The latter case is of special interest from the point of view of CIMS and also for applications in microwave generation and magnetic memories. Both in-plane and out-of-plane components of the torque exerted on both ferromagnetic parts of the junctions have been calculated and shown to be of comparable magnitude. This is in contrast to metallic nanopillars, where the out-of-plane component of the torque is usually much smaller than the in-plane one. In symmetric junctions, the out-of-plane torque is symmetric with respect to bias reversal, whereas the in-plane torque is not symmetric. These conclusions are in agreement with the results obtained by Theodonis *et al.*<sup>[14](#page-8-13)</sup> Both components of the torque are maximal for perpendicular orientation of the electrodes' magnetizations. The spin torque depends not only on the spin splitting of the electron bands in the electrodes but also on the barrier height and thickness. The magnitude of both components of the spin torque normalized to the charge current increases with increasing barrier height and decreases with increasing barrier thickness. In junctions with very low and (or) wide barrier, both components of the torque can change sign.

In turn, the spin torque in junctions with a very thin ferromagnetic layer is shown to oscillate with the thickness of this thin layer, which is a consequence of the quantum spinwell effects. Moreover, it has been shown that the torque may change sign when the thickness of the ferromagnetic layer is varied.

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