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Spin-dependent transmission coefficients for magnetic tunnel junctions: Transport properties and temperature dependence

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In this paper we present a detailed analysis of the spin-dependent transmission coefficients for magnetic tunnel junctions (MTJ's) including magnon scattering dependence. The conduction electrons are modeled as plane waves and the electron-magnon interaction in the interfaces can be treated as a perturbation opening the spin-flip conduction channels. We explore the main transport properties of the MTJ such as bias and temperature dependence of conductance and magnetoresistance. Our theory is in good agreement with experimental data.

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I. INTRODUCTION

Nowadays, the interest on the phenomena of giant magnetoresistance (GMR) in magnetic tunnel junctions (MTJ's) has grown significantly due to potential applications in magnetoresistive reading heads, magnetic field sensors, nonvolatile magnetic random access memories, and many others.^{1–5} The effect is based on the spin-dependent scattering mechanisms proposed in the early papers by Cabrera and Falicov,⁶ which lead in MTJ's, to a strong dependence of the conductance on the magnetic polarization.⁷ A model for spin tunneling was formulated by Jullière⁷ and later developed by Stearns⁸ and Slonczewski.⁹ Typically, the GMR effect found in MTJ's is of the order of 25–30 %,^{10,11} and points to a large ratio of the densities of states for majority (*M*) and minority (*m*) electrons at the Fermi level (*E_F*)

$$\frac{N_M(E_F)}{N_m(E_F)} \approx 2.0-2.5.$$

As usual in MR experiments, one compares the resistances for the cases where the magnetizations at the electrodes are antiparallel (AP) and parallel (P). In several experiments reported in the literature (see, for example, Refs. 1, 2, 10, and 11), the junction resistance drops significantly with the applied voltages, with a sharp peak at zero bias (zero-bias anomaly). This bias dependence shows a rapid initial decrease up to voltages of the order of $V \sim 100$ mV, then slows down but continues decreasing with voltages, up to 60% of the peak value at 500 mV in some cases.¹¹

In Ref. 10, scattering from magnons at the electrodeinsulator interface has been proposed as the mechanism for randomizing the tunneling process and opening the spin-flip channels that reduce the MR. While this process may explain the MR behavior in the vicinity of zero-bias (voltages smaller than 40-100 mV), estimations of magnon scattering cross sections show that the effect is too small to account for the sharp drop in resistance observed in the whole range of 500 mV. In fact, inelastic-electron tunneling spectroscopy (IETS) measurements at low temperature showed peaks which can unambiguously be associated with one-magnon spectra at very small voltages (from 12 to 20 mV, with tails up to 40 mV, and maximum magnon energy not larger than 100 meV).¹ To go beyond this limit will imply multimagnon processes, which are negligible at low temperature. This way, the electron-magnon coupling constant coming from Ref. 10 is by sure considerable overestimated.

The above explanation¹⁰ has been challenged in Ref. 12, where it is shown that the experimental data can be understood in terms of elastic tunneling currents which conserve spin, by considering effects not taken into account in Ref. 10. Those include the lowering of the effective barrier height with the applied voltage, as in the classical Simmons' theory,¹³ and most important, variations of the densities of states with the bias at both magnetic electrodes. The latter is a relevant question, since experiments probe depths of the order of 0.5 eV from the Fermi surface. The bias dependence of MR due to the electronic structure of tunneling junctions has been discussed in Ref. 14 and a simple calculation developed in Ref. 12 models the band structure with free electronlike densities of states, since the tunneling current is dominated by the s-electron contribution. This approach yields a zero bias anomaly which depends on the band structure, and a variation of the MR which has the right order of magnitude for the whole range of 500 meV. The above discussion and other experimental results primarily exhibit that the density of states dependence on the applied voltage plays an important role.^{14–16} However, fine details of experiments at very small voltages are difficult to fit. One may adopt here a pragmatic procedure, with a more intricate band structure and more free parameters to improve the fitting.² Many works take a different stand, motivated by results from IETS experiments.¹ In Ref. 17 the simple model set forth by Bratkovsky¹⁸ with the addition of many-body effects is used, showing that the coupling of electrons to magnetic excitations is very important. The minority electrons are considered as quasiparticles by virtue of their strong coupling to spin waves. In Ref. 19 a consistent study of the voltage dependence of the "giant" magnetoresistance in ferromagnetic tunneling junctions is presented. The main transport properties at low bias and temperatures near 0 K were well established, including the lowering of the effective barrier height with the applied voltage, different variations of the density of states for each spin band with voltage and magnon assisted inelastic tunneling near zero bias. Taking into account all those effects is essential to fully explain experimental results at low temperature for the voltage range between 0 and 500 mV. However, in that work the direct and inelastic transmission coefficients are assumed to be given by a simple WKB approximation and the temperature dependence is not analyzed. Temperature dependence of conductance and MR were investigated by various works.^{3,11,20}

In Ref. 21 the spin dependence of the inelastic mean free path and electronic structure of electrons at low temperatures in transition ferromagnetic metals is explored, considering excited electrons as plane waves. While in bulk ferromagnet the mean free path is important in the evaluation of transport properties such as the conductance in the tunneling phenomena the main contribution comes from s electrons, that can be considered as plane waves.

In this paper our aim is to give a detailed analysis of the tunneling transmission coefficients in a magnetic tunnel junction including the electron-magnon scattering dependence. We consider that the electrons tunneling through the barrier are s-like in the ferromagnetic electrodes, being modeled by plane waves. Magnons are present in the ferromagnet-insulator interfaces and the electron-magnon interaction can be treated as a perturbation responsible for the opening of spin-flip conduction channels. The interfaces are assumed to be perfect and there are no impurity scattering centers inside the barrier. That situation correspond to a perfect MTJ. Otherwise the transport properties are asymmetric with respect to the applied voltage. The transfer matrix method is used to obtain the transmission coefficients. After that, the main transport properties such as bias and temperature dependence of conductance and magnetoresistance can be obtained. A complete theory should then include the following.

(i) A detailed analysis of the spin-dependent transmission coefficients which lead to lowering of the effective barrier height with the applied voltage and magnon scattering dependence of the spin-flip transmission coefficients. We assume that the tunneling electrons are mainly of *s*-character represented by plane waves.

(ii) Magnon assisted tunneling effects, with maximum magnon energies of the order of ~ 100 meV. At low temperature, electrons from the electrodes, accelerated by the applied voltage, excite magnons at the interface. At low temperature, only magnon-emission processes should be considered.

(iii) Variation with voltages of the densities of states for the different spin bands in the ferromagnets. Here, we will follow closely the approach of Refs. 12 and 19, with a simple picture of the band structure. This is motivated by the discussions given in Refs. 12 and 15 over the polarization of the tunneling current.

The content of this paper can be described as follows. In the next section, we put forward the theoretical model, giving a general description of the FM-IS-FM structure and proposing the Hamiltonian and its general solutions. In Sec. III we obtain the spin-dependent tunneling coefficients through the use of the transfer matrix method. Section IV presents a study of the MTJ transport properties and in the last section, a few conclusions and remarks are added.



FIG. 1. A typical magnetic tunnel junction: FM_I and FM_{II} are two ferromagnetic electrodes, TR_I and TR_{II} are also ferromagnetic but there the magnetization is permitted to rotate, due to the presence of magnons. IS is a potential barrier provided by a thin oxide film.

II. THEORETICAL FRAMEWORK

A typical magnetic tunnel junction is shown in Fig. 1. The semi-infinite regions FM_I and FM_{II} are two metallic ferromagnetic electrodes with the magnetization strongly oriented along the z direction, provided by the alignment of the spin of *d* electrons. Notice that the direction of the magnetization corresponds to the direction of spin quantization and we could have chosen the x or y direction to be the direction of the magnetization. The following analysis is not affected by the choice of a particular direction of quantization, that only imply the choice of the most appropriate spin basis. It is shown experimentally through IETS (Ref. 11) that spin wave excitations (magnons) occur close to the interfaces FM-IS (surface magnons). So, we considered into the ferromagnetic reservoirs transition regions, denominated TR_I and TR_{II}, where the direction of the magnetization is rotated and the existence of magnons is allowed. When the magnon wave vector **q** is quasi-two-dimensional the magnon wave function is localized at the interfaces, but with finite localization length and we have thin transition regions. The above discussion can be viewed classically as a consequence of the Maxwell equation $\nabla \cdot \mathbf{B} = \mu_0 \nabla (\mathbf{H} + \chi \mathbf{M}) = 0$. For ferromagnetic materials $\chi \ge 1$, $\mathbf{B} \approx \mu_0 \chi \mathbf{M}$ and $\mathbf{M} = M\hat{z}$ in the semiinfinite reservoirs. However, the medium discontinuity (from ferromagnetic metal to nonferromagnetic insulator) permits the vector M to rotate in the transition regions close to the interfaces. The transition regions allow spin-flip of the incoming and outgoing electron through electron-magnon interaction as will be seen later. The region named IS is a nonferromagnetic insulator representing a potential barrier, where the conduction electron is not subjected to magnetic interactions, i.e., there are no spin interaction inside the barrier. In practice the insulator is made of a thin oxide film. To describe the abovementioned we follow Refs. 9 and 18 and decompose the total Hamiltonian into five parts:

$$H_1 = \frac{\mathbf{p}^2}{2m} - \Delta_1 \sigma_z \quad (-\infty \le z \le -\delta), \tag{1}$$

$$H_2 = \frac{\mathbf{p}^2}{2m} - g \int d^3 x' J(\mathbf{x}, \mathbf{x}') \vec{\sigma} \cdot \mathbf{S}_1(\mathbf{x}') \quad (-\delta \le z \le 0),$$
(2)

$$H_3 = \frac{\mathbf{p}^2}{2m} + V_0 \quad (0 \le z \le d), \tag{3}$$

$$H_4 = \frac{\mathbf{p}^2}{2m} - g \int d^3 x' J(\mathbf{x}, \mathbf{x}') \vec{\sigma} \cdot \mathbf{S}_2(\mathbf{x}') \quad (d \le z \le d + \delta),$$
(4)

$$H_5 = \frac{\mathbf{p}^2}{2m} - \Delta_2 \sigma_z \quad (d + \delta \le z \le +\infty), \tag{5}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ stands for the Pauli spin matrices. Δ_1 and Δ_2 are related to the electron's interaction with the magnetization provided by *d* electrons in each ferromagnetic electrode. $J(\mathbf{x}, \mathbf{x}')$ represents the exchange between *s* and *d* electrons and *g* is some coupling constant between conduction electrons and the magnon fields \mathbf{S}_1 and \mathbf{S}_2 in the transition regions. δ is the effective thickness of the transition regions. V_0 is the effective barrier height and *d* its thickness. The spin wave excitations are described by a linearized Holstein-Primakoff transformation²²

$$\mathbf{S} = \sqrt{2S/N} \sum_{\mathbf{q}} \left(e^{-i\mathbf{q}\cdot\mathbf{x}} b_{\mathbf{q}} \hat{e}_{+} + e^{i\mathbf{q}\cdot\mathbf{x}} b_{\mathbf{q}}^{\dagger} \hat{e}_{-} \right) + \left(S - 1/N \sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{x}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}'} \right) \hat{e}_{z}$$
(6)

being *N* the number of sites at the interface, *S* the spin, $b_{\mathbf{q}}$ and $b_{\mathbf{q}}^{\dagger}$ the annihilation and creation magnon operators with wave vector \mathbf{q} , $\hat{e}_{+}(\hat{e}_{-})$ the positive (negative) helicity of the magnon. The number of magnons is given by the Bose-Einstein distribution $n_{\mathbf{q}}=1/[\exp(\hbar\omega_{\mathbf{q}}/k_{B}T)-1]$, being *T* the absolute temperature and k_{B} the Boltzmann constant. In the spirit of a one-magnon theory we neglect two magnon scattering processes and when $N \ge n_{\mathbf{q}}=b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}$ we may write approximately

$$\mathbf{S} = \sqrt{2S/N} \sum_{\mathbf{q}} \left(e^{-i\mathbf{q}\cdot\mathbf{x}} b_{\mathbf{q}} \hat{e}_{+} + e^{i\mathbf{q}\cdot\mathbf{x}} b_{\mathbf{q}}^{\dagger} \hat{e}_{-} \right) + S \hat{e}_{z}.$$
 (7)

The unperturbed magnetic Hamiltonian is written as follows:

$$H_{0M} = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}.$$
 (8)

The Hamiltonians (1) and (5) are diagonal in the σ_z basis and have identical solutions. The general form $(\mathbf{p}^2/2m - \Delta \sigma_z)\Psi = E\Psi$ has the following solutions:

$$\Psi_{\uparrow} = e^{\pm ik_{\uparrow}z}\chi_{\uparrow}, \qquad (9)$$

$$\Psi_{\downarrow} = e^{\pm i k_{\downarrow} z} \chi_{\downarrow}, \qquad (10)$$

where $k_{\uparrow} = \sqrt{2m(E+\Delta)}/\hbar$ and $k_{\downarrow} = \sqrt{2m(E-\Delta)}/\hbar$, χ_{σ} are the Pauli spinors

$$\chi_{\uparrow} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
 and $\chi_{\downarrow} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ (11)

and the sign + (-) in the exponential must be chosen for an electron with positive (negative) velocity along the *z* axis.

For the Hamiltonians (2) and (4) the general form is $H = \mathbf{p}^2/2m - g \int d^3x' J(\mathbf{x}, \mathbf{x}') \vec{\sigma} \cdot \mathbf{S}(\mathbf{x}')$, which is nondiagonal in the σ_z basis. The Pauli spin matrices can be represented by $\vec{\sigma} = (\sigma^+, \sigma^-, \sigma^z)$, with $\sigma^{\pm} = \sigma^x \pm i\sigma^y$ and whose action on the Pauli spinors are the raising (lowering) of the spin:

$$\sigma^+ \chi_\sigma = \delta_{\sigma \downarrow} \chi_\uparrow$$
 and $\sigma^- \chi_\sigma = \delta_{\sigma \uparrow} \chi_\downarrow$,

 $\delta_{\sigma\sigma'}$ is the Kronecker delta function. The Hamiltonians (2) and (4) in transition regions in terms of the quantized magnon field is written below:

$$\begin{split} H &= \frac{\mathbf{p}^2}{2m} - gS\Delta\sigma^z - g\sqrt{2S/N}\sum_{\mathbf{q}} \int d^3x' J(\mathbf{x},\mathbf{x}')(e^{-i\mathbf{q}\cdot\mathbf{x}'}b_{\mathbf{q}}\sigma^- \\ &+ e^{i\mathbf{q}\cdot\mathbf{x}'}b_{\mathbf{q}}^{\dagger}\sigma^+), \end{split}$$

with $\Delta = \int d^3x' J(\mathbf{x}, \mathbf{x}')$ constant and $S^z = S\Delta$. Notice that the product of circular unitary vectors are $\hat{e}_{\pm} \cdot \hat{e}_{\mp} = 1$ and $\hat{e}_{\pm} \cdot \hat{e}_{\pm} = 0$. For that reason the term σ^+ of the electron spin is combined with the magnon creation term. It means that a magnon with negative angular momentum is created while the electron changes its spin from down to up state, conserving the angular momentum of the whole system. Making the following definition:

$$f(\mathbf{x},\mathbf{q}) = \int d^3x' J(\mathbf{x},\mathbf{x}') e^{-i\mathbf{q}\cdot\mathbf{x}'},$$

the Hamiltonian takes a simpler form

$$H = \frac{\mathbf{p}^{z}}{2m} - gS^{z}\sigma^{z} - g\sqrt{2S/N}\sum_{\mathbf{q}} \left[f(\mathbf{x},\mathbf{q})b_{\mathbf{q}}\sigma^{-} + f^{*}(\mathbf{x},\mathbf{q})b_{\mathbf{q}}^{\dagger}\sigma^{+}\right].$$
(12)

Now, we will calculate the electron wave function through the use of the perturbation theory, with the magnon field as the perturbation

$$H_0 = \frac{\mathbf{p}^2}{2m} - gS^z \sigma^z, \tag{13}$$

$$H_I = -g\sqrt{2S/N}\sum_{\mathbf{q}} \left[f(\mathbf{x},\mathbf{q})b_{\mathbf{q}}\sigma^- + f^*(\mathbf{x},\mathbf{q})b_{\mathbf{q}}^{\dagger}\sigma^+\right].$$
(14)

The interaction Hamiltonian (14) makes the transition of magnon states with different magnon numbers in the Fock space. The overall solution is a tensor product of the magnon's wave function with the electron's wave function. The eigenkets which make both Hamiltonians (8) and (13) diagonal simultaneously are $\{|\mathbf{k}, \sigma\rangle \otimes |n_q\rangle\} = \{|\mathbf{k}, \sigma; n_q\rangle\}$. However, we are interested only in obtaining the electron's wave function and the magnon states will be omitted. To the first order the perturbation theory yields

$$|\Psi^{+}\rangle = |\Psi_{\uparrow}\rangle + \frac{\langle\Psi_{\downarrow}|H_{I}|\Psi_{\uparrow}\rangle}{E_{\uparrow} - E_{\downarrow}}|\Psi_{\downarrow}\rangle$$

$$\left|\Psi^{-}\right\rangle = \left|\Psi_{\downarrow}\right\rangle + \frac{\left\langle\Psi_{\uparrow}\right|H_{I}|\Psi_{\downarrow}\right\rangle}{E_{\perp} - E_{\uparrow}}\left|\Psi_{\uparrow}\right\rangle$$

being $E_{\uparrow} - E_{\downarrow} = -2gS^z = -2g\Delta S$. We write the solutions explicitly, as follows:

$$|\Psi^{+}\rangle = |\Psi_{\uparrow}\rangle + \frac{f(\mathbf{q})\sqrt{n_{\mathbf{q}}}}{\sqrt{2S\Delta N}}|\Psi_{\downarrow}\rangle, \qquad (15)$$

$$|\Psi^{-}\rangle = |\Psi_{\downarrow}\rangle - \frac{f^{*}(\mathbf{q})\sqrt{n_{\mathbf{q}}+1}}{\sqrt{2S\Delta N}}|\Psi_{\uparrow}\rangle.$$
(16)

The functions (15) and (16), normalized with respect to the first order approximation, are the general solutions of the Hamiltonians (2) and (4). At low temperatures $n_q \rightarrow 0$ and these solutions are written as follows:

$$|\Psi^{+}\rangle = |\Psi_{\uparrow}\rangle, \tag{17}$$

$$|\Psi^{-}\rangle = |\Psi_{\downarrow}\rangle - \frac{f^{*}(\mathbf{q})}{\sqrt{2S\Delta N}}|\Psi_{\uparrow}\rangle.$$
(18)

Looking at them the obvious conclusion is that the spin up state $(|\Psi_{\uparrow}\rangle)$ will not interact with the magnon field while the spin down state $(|\Psi_{\downarrow}\rangle)$ interact with magnon field by emission process. At higher temperatures $n_q \neq 0$ and magnon emission and absorption processes are allowed. Thus, the electron's wave functions can be represented by

$$|\Psi^{+}\rangle = \sin \alpha |\Psi_{\uparrow}\rangle + \cos \alpha e^{-i\phi} |\Psi_{\downarrow}\rangle, \qquad (19)$$

$$|\Psi^{-}\rangle = \cos \alpha |\Psi_{\uparrow}\rangle - \sin \alpha e^{-i\phi} |\Psi_{\downarrow}\rangle.$$
 (20)

This case is being analyzed in another paper,²³ where the effective magnetization is represented by the angle α .

Finally, in the barrier Hamiltonian (3) we do not have spin interactions, being the simplest solution written below

$$\Psi = (A\chi_{\uparrow} + B\chi_{\downarrow})e^{\gamma z} + (C\chi_{\uparrow} + D\chi_{\downarrow})e^{-\gamma z}$$
(21)

with $\gamma = \sqrt{2m(V_0 - E)}/\hbar$, $V_0 > E$. Now we know the general solutions of the Hamiltonians (1)–(5), each one representing one of the five distinct regions FM_I, TR_I, IS, TR_{II}, and FM_{II}, and we need to match these solutions by making Ψ and $d\Psi/dz$ continuous at the interfaces. This will be done in the next section.

III. THE SPIN-DEPENDENT TRANSMISSION COEFFICIENTS

For the determination of the spin-dependent transmission coefficients in the FM-IS-FM structure the transfer matrix method is the most useful. In the metallic ferromagnetic electrodes the electrons are subjected to inelastic scattering, being the mean free path spin dependent.²¹ However, we are dealing with tunneling and the main contribution to the currents comes from *s* electrons, which can be represented by plane wave solutions. Consider that in region FM_I the electron's wave function is composed by an incident part and a reflected one $\Psi_1 = \Psi_{inc} + \Psi_{refl}$, obeying (9) and (10):

$$\Psi_1 = (I_{\uparrow} e^{ik_{\uparrow}z} + R_{\uparrow} e^{-ik_{\uparrow}z})\chi_{\uparrow} + (I_{\downarrow} e^{ik_{\downarrow}z} + R_{\downarrow} e^{-ik_{\downarrow}z})\chi_{\downarrow}. \quad (22)$$

 I_{\uparrow} (I_{\downarrow}) is the amplitude of the incident wave with spin up (down) and R_{\uparrow} (R_{\downarrow}) is the amplitude of the reflected waves with spin up (down). The wave functions among the two ferromagnetic regions are easily obtained but they will not be shown here. The transmitted wave to the ferromagnetic electrode FM_{II}, propagating forward in the *z* axis is written in the following way:

$$\Psi_t = T_{\uparrow} e^{ik_{\uparrow}' z} \chi_{\uparrow} + T_{\downarrow} e^{ik_{\downarrow}' z} \chi_{\downarrow}$$
(23)

being T_{\uparrow} and T_{\downarrow} the transmission amplitudes for spin up and spin down, respectively. The transfer matrix equation is obtained by requiring the continuity of the function Ψ and its derivative $d\Psi/dz$ in the interfaces, yielding

$$\begin{pmatrix} I_{\uparrow} \\ R_{\uparrow} \\ I_{\downarrow} \\ R_{\downarrow} \end{pmatrix} = M_1 M_2 M_3 M_4 M_5 \begin{pmatrix} T_{\uparrow} \\ 0 \\ T_{\downarrow} \\ 0 \end{pmatrix}$$
(24)

with the matrices M_j , $j=1,2,\ldots,5$ defined below

$$M_{1} = \begin{pmatrix} M_{1\uparrow}^{-1} & 0\\ 0 & M_{1\downarrow}^{-1} \end{pmatrix},$$
(25)

where 0 is the 2×2 null matrix and

$$M_{1\uparrow} = \begin{pmatrix} e^{-ik_{\uparrow}\delta} & e^{ik_{\uparrow}\delta} \\ ik_{\uparrow}e^{-ik_{\uparrow}\delta} & -ik_{\uparrow}e^{ik_{\uparrow}\delta} \end{pmatrix},$$

$$M_{1\downarrow} = \begin{pmatrix} e^{-ik_{\downarrow}\delta} & e^{ik_{\downarrow}\delta} \\ ik_{\downarrow}e^{-ik_{\downarrow}\delta} & -ik_{\downarrow}e^{ik_{\downarrow}\delta} \end{pmatrix},$$

$$M_{2} = \begin{pmatrix} b_{1}c_{1}A + b_{2}c_{3}B & b_{1}c_{2}A + b_{2}c_{4}B \\ b_{3}c_{1}A + b_{4}c_{3}B & b_{3}c_{2}A + b_{4}c_{4}B \end{pmatrix},$$
(26)

where

$$A = \begin{pmatrix} \cos(k_+\delta) & -(k_+)^{-1}\sin(k_+\delta) \\ k_+\sin(k_+\delta) & \cos(k_+\delta) \end{pmatrix}$$

and

$$B = \begin{pmatrix} \cos(k_{-}\delta) & -(k_{-})^{-1}\sin(k_{-}\delta) \\ k_{-}\sin(k_{-}\delta) & \cos(k_{-}\delta) \end{pmatrix},$$
$$M_{3} = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix}, \text{ where } C$$
$$= \begin{pmatrix} \cosh(\gamma d) & -\gamma^{-1}\sinh(\gamma d) \\ -\gamma\sinh(\gamma d) & \cosh(\gamma d) \end{pmatrix}, \qquad (27)$$

$$M_{4} = \begin{pmatrix} b_{1}c_{1}A' + b_{2}c_{3}B' & b_{1}c_{2}A' + b_{2}c_{4}B' \\ b_{3}c_{1}A' + b_{4}c_{3}B' & b_{3}c_{2}A' + b_{4}c_{4}B' \end{pmatrix},$$
(28)

where

$$A = \begin{pmatrix} \cos(k'_{+}\delta) & -(k'_{+})^{-1}\sin(k_{+}\delta) \\ k'_{+}\sin(k'_{+}\delta) & \cos(k'_{+}\delta) \end{pmatrix}$$

and

$$B = \begin{pmatrix} \cos(k'_{-}\delta) & -(k'_{-})^{-1}\sin(k'_{-}\delta) \\ k'_{-}\sin(k'_{-}\delta) & \cos(k'_{-}\delta) \end{pmatrix},$$
$$M_{5} = \begin{pmatrix} M_{5\uparrow} & 0 \\ 0 & M_{5\downarrow} \end{pmatrix},$$
$$M_{5\uparrow} = \begin{pmatrix} e^{ik'_{\uparrow}(d+\delta)} & 0 \\ ik'_{\uparrow}e^{ik'_{\uparrow}(d+\delta)} & 0 \end{pmatrix}, \quad M_{5\downarrow} = \begin{pmatrix} e^{ik'_{\downarrow}(d+\delta)} & 0 \\ ik'_{\downarrow}e^{ik'_{\downarrow}(d+\delta)} & 0 \end{pmatrix}.$$
(29)

The parameters b_i and c_i depend on the magnon field through $f(\mathbf{q})$ and $n(\mathbf{q})$. They are defined below:

$$b_{1} = \frac{1}{N^{+}}, \quad b_{2} = \frac{-f^{*}(\mathbf{q})\sqrt{n_{\mathbf{q}}+1}}{N^{-}\sqrt{2N|\Delta|S}},$$
$$b_{3} = \frac{f(\mathbf{q})\sqrt{n_{\mathbf{q}}}}{N^{+}\sqrt{2N|\Delta|S}}, \quad b_{4} = \frac{1}{N^{-}},$$
(30)

$$c_{1} = N^{+} \left(1 + \frac{|f(\mathbf{q})|^{2} \sqrt{n_{\mathbf{q}}(n_{\mathbf{q}}+1)}}{2N|\Delta|S} \right)^{-1},$$

$$c_{2} = N^{+} \left(\frac{\sqrt{2N|\Delta|S}}{f^{*}(\mathbf{q})\sqrt{n_{\mathbf{q}}+1}} + \frac{f(\mathbf{q})\sqrt{n_{\mathbf{q}}}}{\sqrt{2N|\Delta|S}} \right)^{-1},$$

$$c_{3} = N^{-} \left(\frac{f^{*}(\mathbf{q})\sqrt{n_{\mathbf{q}}+1}}{\sqrt{2N|\Delta|S}} + \frac{\sqrt{2N|\Delta|S}}{f(\mathbf{q})\sqrt{n_{\mathbf{q}}}} \right)^{-1},$$

$$c_{4} = N^{-} \left(1 + \frac{|f(\mathbf{q})|^{2}\sqrt{n_{\mathbf{q}}(n_{\mathbf{q}}+1)}}{2N|\Delta|S} \right)^{-1}$$
(31)

with $N^+ = \sqrt{1 + n_{\mathbf{q}} |f(\mathbf{q})|^2 / (2N|\Delta|S)}$ and $N^- = \sqrt{1 + (n_{\mathbf{q}} + 1) |f(\mathbf{q})|^2 / (2N|\Delta|S)}$.

Equation (24) allowed us to directly determine T_{\uparrow} and T_{\downarrow} as functions of the incident amplitudes I_{\uparrow} and I_{\downarrow} and the *M* matrix elements M_{ij} . One can easily show that

$$T_{\uparrow} = \frac{M_{33}I_{\uparrow} - M_{13}I_{\downarrow}}{M_{11}M_{33} - M_{13}M_{31}}$$
(32)

and

$$T_{\downarrow} = \frac{M_{11}I_{\downarrow} - M_{31}I_{\uparrow}}{M_{11}M_{33} - M_{13}M_{31}}.$$
 (33)

However, now we will define more appropriate coefficients, considering that the incident electron is only spin up (only spin down), which means $I_{\uparrow} \neq 0$ and $I_{\downarrow} = 0$ ($I_{\uparrow} = 0$ and $I_{\downarrow} \neq 0$). The new amplitudes are defined below:

$$T_{\uparrow\uparrow} = \frac{T_{\uparrow}}{I_{\uparrow}} = \frac{M_{33}}{M_{11}M_{33} - M_{13}M_{31}},$$
(34)

$$T_{\uparrow\downarrow} = \frac{T_{\downarrow}}{I_{\uparrow}} = \frac{-M_{31}}{M_{11}M_{33} - M_{13}M_{31}},$$
 (35)

$$T_{\downarrow\uparrow} = \frac{T_{\uparrow}}{I_{\downarrow}} = \frac{-M_{13}}{M_{11}M_{33} - M_{13}M_{31}},$$
(36)

$$T_{\downarrow\downarrow} = \frac{T_{\downarrow}}{I_{\downarrow}} = \frac{M_{11}}{M_{11}M_{33} - M_{13}M_{31}}.$$
 (37)

The meaning of the coefficients (34)–(37) is described as follows: $T_{\uparrow\uparrow}$ is the probability amplitude of a spin up incident electron to be transmitted through the barrier without spin flip, while $T_{\uparrow\downarrow}$ is the probability amplitude of a spin up electron to be transmitted flipping its spin. An analogous explanation follows for a spin down incident electron, being the amplitudes given by $T_{\downarrow\uparrow}$ for flipping its spin in the tunneling and $T_{\downarrow\downarrow}$ for conserving its spin. The exact expressions resulting from the above are very complicated. Instead of showing them we will proceed taking the limit of low temperatures, that implicates in $n_{\mathbf{q}} \rightarrow 0$ and some simplifications take place. In fact, when $n_{\mathbf{q}} \rightarrow 0$ we have $b_3=c_2=c_3=0$, $b_1c_1=b_4c_4=1$, $b_2c_4=\alpha=-f^*(\mathbf{q})/\sqrt{2N|\Delta|S}$ and we put the matrices M_2 and M_4 in the following form:

$$M_2 = \begin{pmatrix} A & \alpha B \\ 0 & B \end{pmatrix}, \quad M_4 = \begin{pmatrix} A' & \alpha B' \\ 0 & B' \end{pmatrix}.$$
 (38)

When surface magnons must be considered the dimension δ must be small compared to the barrier effective thickness, and another approximation can be made, i.e., we can expand the matrices A, A', B, B' in $k\delta \rightarrow 0$. Then after a bit of algebra the final result $M = M_1 M_2 M_3 M_4 M_5$ is

$$M = \begin{pmatrix} M_{1\uparrow}^{-1}CM_{5\uparrow} & 2\alpha M_{1\uparrow}^{-1}CM_{5\downarrow} \\ 0 & M_{1\downarrow}^{-1}CM_{5\downarrow} \end{pmatrix} + \delta \begin{pmatrix} M_A C + CM_{A'} & \alpha (M_A + M_{B'})C + 2\alpha CM_{B'} \\ 0 & M_B CM_{B'} \end{pmatrix} + O(\delta^2), \qquad (39)$$

where M_A , $M_{A'}$, M_B and $M_{B'}$ the residual matrices of A, A', B and B', respectively, coming from the approximation $k\delta \rightarrow 0$. We wrote them below:

$$M_{A} = \begin{pmatrix} 0 & -1 \\ (k_{+})^{2} & 0 \end{pmatrix}, \quad M_{B} = \begin{pmatrix} 0 & -1 \\ (k_{-})^{2} & 0 \end{pmatrix},$$
$$M_{A'} = \begin{pmatrix} 0 & -1 \\ (k'_{+})^{2} & 0 \end{pmatrix}, \quad M_{B'} = \begin{pmatrix} 0 & -1 \\ (k'_{-})^{2} & 0 \end{pmatrix}.$$

Keeping terms to the zero order, i.e., neglecting the δ term, we have

$$M_{11} = \frac{1}{2} e^{ik_{\uparrow}'} \left[\left(1 + \frac{k_{\uparrow}'}{k_{\uparrow}} \right) \cosh(\gamma d) + i \left(\frac{\gamma}{k_{\uparrow}} - \frac{k_{\uparrow}'}{\gamma} \right) \sinh(\gamma d) \right],$$
$$M_{13} = \alpha e^{ik_{\downarrow}'} \left[\left(1 + \frac{k_{\downarrow}'}{k_{\uparrow}} \right) \cosh(\gamma d) + i \left(\frac{\gamma}{k_{\uparrow}} - \frac{k_{\downarrow}'}{\gamma} \right) \sinh(\gamma d) \right],$$

$$M_{33} = 0$$

$$M_{33} = \frac{1}{2}e^{ik_{\perp}'} \left[\left(1 + \frac{k_{\perp}'}{k_{\perp}} \right) \cosh(\gamma d) + i \left(\frac{\gamma}{k_{\perp}} - \frac{k_{\perp}'}{\gamma} \right) \sinh(\gamma d) \right].$$

M = 0

We calculated the transmission amplitudes by the formulas (34)–(37). The results are shown below, for the transmission probabilities

$$|T_{\uparrow\uparrow}|^{2} = \frac{4}{\left(1 + \frac{k_{\uparrow}^{\prime 2}}{k_{\uparrow}^{2}}\right)^{2} + \left(\frac{(k_{\uparrow}^{2} + \gamma^{2})(k_{\uparrow}^{\prime 2} + \gamma^{2})}{k_{\uparrow}^{2}\gamma^{2}}\right) \sinh^{2}(\gamma d)},$$
(40)

$$T_{\uparrow\downarrow}|^2 = 0, \tag{41}$$

$$|T_{\downarrow\uparrow}|^{2} = \frac{|f(\mathbf{q})|^{2}|T_{\uparrow\uparrow}|^{2}|T_{\downarrow\downarrow}|^{2}}{2N|\Delta|S} \left[\left(1 + \frac{k_{\downarrow}^{\prime 2}}{k_{\uparrow}^{2}}\right)^{2} + \left(\frac{(k_{\uparrow}^{2} + \gamma^{2})(k_{\downarrow}^{\prime 2} + \gamma^{2})}{k_{\uparrow}^{2}\gamma^{2}}\right) \sinh^{2}(\gamma d) \right], \quad (42)$$

$$|T_{\downarrow\downarrow}|^{2} = \frac{4}{\left(1 + \frac{k_{\downarrow}^{\prime 2}}{k_{\downarrow}^{2}}\right)^{2} + \left(\frac{(k_{\downarrow}^{2} + \gamma^{2})(k_{\downarrow}^{\prime 2} + \gamma^{2})}{k_{\downarrow}^{2}\gamma^{2}}\right) \sinh^{2}(\gamma d)}.$$
(43)

The above equations are in absolute agreement with what one could expect intuitively. At low temperatures, only magnon emission is allowed and for this reason it is required that $|T_{\uparrow\downarrow}|^2=0$. The direct tunneling probabilities (conserving spin) are those obtained for a particle without spin²⁴ in an asymmetric barrier, while the magnon-assisted transmission coefficient (flipping spin) is proportional to some function depending on the elctron-magnon coupling $|f(\mathbf{q})|^2/2N|\Delta|S$. Taking into account first-order terms in δ the spin-flip transmission probability will be augmented. For low voltages, the above expressions can be approximated because $\gamma d \ge 1$, yielding

$$|T_{\uparrow\uparrow}|^2 = \frac{16k_{\uparrow}^2\gamma^2}{(k_{\uparrow}^2 + \gamma^2)(k_{\uparrow}'^2 + \gamma^2)} \exp(-2\gamma d), \qquad (44)$$

$$T_{\uparrow\downarrow}|^2 = 0, \tag{45}$$

$$|T_{\downarrow\uparrow}|^{2} = \frac{64|f(\mathbf{q})|^{2}}{2N|\Delta|S} \frac{k_{\downarrow}^{2}\gamma^{2}}{(k_{\downarrow}^{2} + \gamma^{2})(k_{\uparrow}^{\prime 2} + \gamma^{2})} \exp(-2\gamma d), \quad (46)$$

$$|T_{\downarrow\downarrow}|^{2} = \frac{16k_{\downarrow}^{2}\gamma^{2}}{(k_{\downarrow}^{2} + \gamma^{2})(k_{\downarrow}^{\prime 2} + \gamma^{2})} \exp(-2\gamma d).$$
(47)

One can see clearly that the above transmission coefficients are products of the tunneling coefficient for a spin-0 particle with some coupling function and have the same form of that used by Bratkovsky¹⁸ to describe magnetic tunneling junctions. One can find corrective terms by solving the M matrix directly without making approximations. In the analysis we

have considered perfect interfaces and none impurity scattering centers inside the barrier. The obtained coefficients are symmetric with respect to the tunneling from left to right electrode and in the opposite direction. These effects will lead to an asymmetric behavior of the conductance with the applied voltage¹⁷ and/or resonant effects.¹⁸ The transmission coefficients at higher temperatures can be obtained intuitively. To zero-order approximation at a given temperature the magnon number is not zero and absortion processes can occur. In this way we have

$$|T_{\uparrow\uparrow}|^2 = \frac{16k_{\uparrow}^2\gamma^2}{(k_{\uparrow}^2 + \gamma^2)(k_{\uparrow}'^2 + \gamma^2)} \exp(-2\gamma d), \qquad (48)$$

$$|T_{\uparrow\downarrow}|^{2} = \frac{4|f(\mathbf{q})|^{2}n_{\mathbf{q}}}{2N|\Delta|S} \frac{16k_{\uparrow}^{2}\gamma^{2}}{(k_{\uparrow}^{2} + \gamma^{2})(k_{\downarrow}^{\prime 2} + \gamma^{2})} \exp(-2\gamma d), \quad (49)$$

$$|T_{\downarrow\uparrow}|^{2} = \frac{4|f(\mathbf{q})|^{2}(n_{\mathbf{q}}+1)}{2N|\Delta|S} \frac{16k_{\downarrow}^{2}\gamma^{2}}{(k_{\downarrow}^{2}+\gamma^{2})(k_{\uparrow}^{\prime2}+\gamma^{2})} \exp(-2\gamma d),$$
(50)

$$|T_{\downarrow\downarrow}|^{2} = \frac{16k_{\downarrow}^{2}\gamma^{2}}{(k_{\downarrow}^{2} + \gamma^{2})(k_{\downarrow}^{\prime 2} + \gamma^{2})} \exp(-2\gamma d).$$
(51)

In fact, with increasing temperature, corrections to the transmission coefficients are needed. However, the above results can explain the main transport properties in magnetic tunnel junctions with good accuracy. It must be pointed out that $f(\mathbf{q})$ is also a function of \mathbf{k} and \mathbf{k}' , weighted by the exchange integral J(x,x'). The omission is only for sake of convenience.

Another way to understand the above formulae is to write down Feynmann graphs for the processes, but this will not be shown here. The electron interact with the magnon field and with the barrier. To zero order in δ , the electron interact with the surface magnons before transmission or is transmitted directly. The electron-magnon interaction is represented by a coupling function, while for direct transmission the coupling constant is unitary. In the magnon processes we conservation of the overall momentum of the electron-magnon system is a requirement. The interaction with the barrier is always the same as for a particle of spin zero, being the coupling exactly equal to the transmission coefficient, using the appropriate incident and transmitted momentum.

As a last point in this section, it is important to observe that in our formulae only the z component of total momentum of the incident and transmitted electron must be considered. When considering the lattice potential of the ferromagnetic metals the transversal momentum is quantized and the total energy of an electron incident at the interfaces must be weighted by some constant η relating the energy E with its component E_z perpendicular to the barrier by $E_z = \eta E$, as shown in Ref. 25.

IV. THE MAIN TRANSPORT PROPERTIES OF A TYPICAL MTJ

With the spin-dependent transmission coefficients for a typical MTJ in hands, the main transport properties such as

the conductance and magnetoresistance can be easily obtained. The total tunneling current flowing through the junction is given by, quite generally,

$$I = \frac{2\pi e}{\hbar} \int d\epsilon \sum_{\sigma\sigma'} \{ T_{\sigma\sigma'}(\epsilon) N_{\sigma}^{L}(\epsilon - V) N_{\sigma'}^{R}(\epsilon) f_{L}(\epsilon - V) [1 - f_{R}(\epsilon)] - T_{\sigma'\sigma}(\epsilon) N_{\sigma}^{L}(\epsilon - V) N_{\sigma'}^{R}(\epsilon) f_{R}(\epsilon) [1 - f_{L}(\epsilon - V)] \},$$
(52)

where $\epsilon = E - E_F$, E_F is the Fermi energy, $N_{\sigma}^{\alpha}(\epsilon)$ is the density of states for electrons with spin σ , $\alpha = (R, L)$ denote the electrode, and $f(\epsilon) = (\exp[\epsilon/k_BT] + 1)^{-1}$ is the Fermi-Dirac distribution, k_B is the Boltzmann constant, and T is the absolute temperature. The resistance is readily obtained by $R = G^{-1}$, where G = dI/dV is the differential conductance. The magnetoresistance is is defined as

$$\frac{\Delta R}{R} = \frac{R_{\rm AP} - R_P}{R_{\rm AP}}.$$
(53)

Note that the above definition is limited to 100%, since $R_{AP} > R_P$. In the parallel (*P*) configuration the magnetization has the same orientation along the *z* axis for FM_I and FM_{II}, being the majority and minority spin bands the same for both electrodes, while in the antiparallel (AP) scheme, the magnetization of the ferromagnetic electrodes has opposite orientations and, in this case, the majority spin band in FM_I is the minority spin band in FM_{II} and *vice versa*. In the low bias regime, we are interested in voltages smaller than the Fermi energy and only the states near the Fermi level will contribute to the transport, so we can expand the density of states in a Taylor series as follows:

$$N^{\alpha}_{\sigma}(\boldsymbol{\epsilon}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n N^{\alpha}_{\sigma}(\boldsymbol{\epsilon})}{d\boldsymbol{\epsilon}^n} \right|_{\boldsymbol{\epsilon}=0} \boldsymbol{\epsilon}^n.$$
(54)

Taking into account identical electrodes and the low bias regime, we can expand these expressions to first order with good accuracy. The *s* band can be represented by a parabolic dispersion relation and density of states $N_{\sigma} \propto \sqrt{E} - \Delta_{\sigma}$, where $\Delta_{\sigma}(\sigma=\uparrow,\downarrow)$ gives the bottom of the spin band, with $|\Delta_{\uparrow} - \Delta_{\downarrow}| = 2\Delta$, as in Refs. 12 and 18. However, we consider here cases more general than the parabolic dispersion, with the band structure described through the following set of parameters:¹⁹

$$r \equiv \left(\frac{N_M}{N_m}\right)_F,$$

$$\lambda \equiv \left(\frac{dN_M/dE}{dN_m/dE}\right)_F,$$

$$\beta \equiv \left(\frac{1}{N_m}\frac{dN_m}{dE}\right)_F,$$
(55)

with all quantities evaluated at the Fermi level, and m and M stand for minority and majority spin bands, respectively. Now we break the total current (52) into a part not involving spin flip (direct current) and another involving magnon scattering (inelastic current). The direct current for a perfect MTJ (the probabilities for tunneling from right to left side electrode and in the opposite direction are the same) is written as follows:

$$I = \frac{2\pi e}{\hbar} \int_{0}^{V} d\epsilon [T_{\uparrow\uparrow}(\epsilon) N_{\uparrow}^{L}(\epsilon - V) N_{\uparrow}^{R}(\epsilon) + T_{\downarrow\downarrow}(\epsilon) N_{\downarrow}^{L}(\epsilon - V) N_{\downarrow}^{R}(\epsilon)].$$
(56)

The transmission coefficient are given by Eqs. (48) and (51). Substituting $k_{\sigma} = \sqrt{2me(\epsilon - \Delta_{\sigma})/\hbar^2}$ and $\gamma = \sqrt{2me(V_0 - \epsilon)/\hbar^2}$ with $V_0 \ge \Delta_{\sigma}$, we have

$$T_{\uparrow\uparrow} = \frac{16(\Delta_{\uparrow} + \eta\epsilon)}{V_0 \left(1 + \frac{\Delta_{\uparrow} + \Delta_{\uparrow}'}{V_0}\right)} \exp\left[-1.024d\sqrt{V_0}\right] \exp\left[\frac{\eta\epsilon d}{\sqrt{V_0}}\right],$$
$$T_{\downarrow\downarrow} = \frac{16(\Delta_{\downarrow} + \eta\epsilon)}{V_0 \left(1 + \frac{\Delta_{\downarrow} + \Delta_{\downarrow}'}{V_0}\right)} \exp\left[-1.024d\sqrt{V_0}\right] \exp\left[\frac{\eta\epsilon d}{\sqrt{V_0}}\right],$$

where *d* is given in Å and the energies in eV. It was shown in a previous work¹⁹ that when $T_{\uparrow\uparrow}=T_{\downarrow\downarrow}$ we can calculate the ratio of the densities of states *r* at the Fermi level using only the experimental value of $\Delta R/R$ at zero bias

$$r = \frac{1}{1 - \frac{\Delta R}{R}} + \sqrt{\frac{1}{\left(1 - \frac{\Delta R}{R}}\right)^2 - 1}, \quad (57)$$

which does not depend on the barrier parameters. This expression needs a little modification when $T_{\uparrow\uparrow} \neq T_{\downarrow\downarrow}$, and we have

$$r \approx \frac{1 + \Delta_{\downarrow}/\Delta_{\uparrow}}{2\left(1 - \frac{\Delta R}{R}\Big|_{V=0}\right)} + \sqrt{\frac{\left(1 + \Delta_{\downarrow}/\Delta_{\uparrow}\right)^{2}}{\left(1 - \frac{\Delta R}{R}\Big|_{V=0}\right)^{2}} - \frac{\Delta_{\downarrow}}{\Delta_{\uparrow}}}.$$
(58)

However, we will not take into consideration these corrections in the direct current and we consider $\Delta_{\downarrow}/\Delta_{\uparrow} \approx 1$, being the final result for the direct conductance at T = 0K

$$G_{d}^{(P)} = \frac{2\pi e^{2}}{\hbar} \exp\left[-1.024d\sqrt{\Phi_{0}}\right] \left[N_{m}^{F}\right]^{2} \left((1+r^{2})\exp\left[\frac{\eta V d}{2\sqrt{\Phi_{0}}}\right] + \frac{\beta(1+r\lambda)}{3} \left\{\frac{\eta dV^{2}}{4\sqrt{\Phi_{0}}}\exp\left[\frac{\eta V d}{2\sqrt{\Phi_{0}}}\right] + V\left(\exp\left[\frac{\eta V d}{2\sqrt{\Phi_{0}}}\right] - 1\right)\right\} - \frac{\beta^{2}(1+\lambda^{2})}{2} \exp\left[\frac{3\eta V d}{10\sqrt{\Phi_{0}}}\right] \left(V^{2} + \frac{\eta V^{3} d}{10\sqrt{\Phi_{0}}}\right)\right)$$
(59)

and

$$\begin{aligned} G_d^{(AP)} &= \frac{2\pi e^2}{\hbar} \exp\left[-1.024d\sqrt{\Phi_0}\right] \left[N_m^F\right]^2 \left\{ 2r \exp\left[\frac{\eta V d}{2\sqrt{\Phi_0}}\right] \right. \\ &+ \frac{\beta(r+\lambda)}{3} \left\{ \frac{\eta dV^2}{4\sqrt{\Phi_0}} \exp\left[\frac{\eta V d}{2\sqrt{\Phi_0}}\right] \right. \\ &+ V \left(\exp\left[\frac{\eta V d}{2\sqrt{\Phi_0}}\right] - 1 \right) \right\} \\ &- \beta^2 \lambda \exp\left[\frac{3\eta V d}{10\sqrt{\Phi_0}}\right] \left(V^2 + \frac{\eta V^3 d}{10\sqrt{\Phi_0}}\right) \right\}. \end{aligned}$$
(60)

Now we will analyze the magnon-assisted tunneling to investigate the zero-bias anomaly and the temperature dependence. The transmission coefficients (49) and (50), in energy variables, are written in the following way:

$$\begin{split} T_{\uparrow\downarrow} &= \rho(\omega,\epsilon) \frac{n(\omega)}{N|\Delta|S} \frac{16(\Delta_{\uparrow} + \eta\epsilon)}{V_0 \left(1 + \frac{\Delta_{\uparrow} + \Delta_{\downarrow}'}{V_0}\right)} \\ &\times \exp[-1.024d\sqrt{V_0}] \exp\left[\frac{\eta\epsilon d}{\sqrt{V_0}}\right], \\ T_{\downarrow\uparrow} &= \rho(\omega,\epsilon) \frac{n(\omega) + 1}{N|\Delta|S} \frac{16(\Delta_{\downarrow} + \eta\epsilon)}{V_0 \left(1 + \frac{\Delta_{\downarrow} + \Delta_{\uparrow}'}{V_0}\right)} \\ &\times \exp[-1.024d\sqrt{V_0}] \exp\left[\frac{\eta\epsilon d}{\sqrt{V_0}}\right], \end{split}$$

where $\rho(\omega, \epsilon) = 2|f(\omega, \epsilon)|^2 g(\omega)$ is the magnon density of states. The parameter $g(\omega)$ is related to the Jacobian of the transformation of the sum on all the magnon wave vectors **q** allowed to an integral on the magnon energy ω , $n(\omega) = (\exp[\omega/k_BT] - 1)^{-1}$ is the magnon number, given by the Bose-Einstein distribution. The emission and absortion currents are written as follows:

$$\begin{split} I_{\rm em} &= \frac{2\pi e}{\hbar} \int d\epsilon \int d\omega \{ T_{\downarrow\uparrow'}(\epsilon) N_{\downarrow}^{L}(\epsilon - V + \omega) N_{\uparrow}^{R}(\epsilon) \\ &\times f_{L}(\epsilon - V + \omega) [1 - f_{R}(\epsilon)] - T_{\downarrow'\uparrow}(\epsilon) N_{\uparrow}^{L}(\epsilon - V + \omega) N_{\downarrow}^{R}(\epsilon) \\ &\times f_{R}(\epsilon + V - \omega) [1 - f_{L}(\epsilon)] \}, \end{split}$$
(61)

$$I_{abs} = \frac{2\pi e}{\hbar} \int d\epsilon \int d\omega \{ T_{\uparrow\downarrow'}(\epsilon) N_{\uparrow}^{L}(\epsilon - V + \omega) N_{\downarrow}^{R}(\epsilon) \\ \times f_{L}(\epsilon - V + \omega) [1 - f_{R}(\epsilon)] - T_{\uparrow'\downarrow}(\epsilon) N_{\downarrow}^{L}(\epsilon - V + \omega) N_{\uparrow}^{R}(\epsilon) \\ \times f_{R}(\epsilon + V - \omega) [1 - f_{L}(\epsilon)] \}.$$
(62)

Neglecting the temperature effects on the Fermi-Dirac distributions they become steplike functions. We consider that both the density of states and the transmission coefficients are constant in the integration interval and take the derivative with respect to the applied voltage V to obtain the conductance. One can use as the magnon dispersion relation a simple isotropic parabolic dependence, i.e., $\hbar \omega = E_m (q/q_m)^2$, where E_m is related to the Curie temperature by the mean-

field approximation $E_m = 3k_B T_C/(S+1)$, and q_m is the radius of the first Brillouin zone.¹⁰ In other words E_m is the maximum magnon energy (high energy cutoff).¹ However, we have considered for the magnon density of states a general expression of the form $\rho(\omega) = a\omega^n \exp[-b(\omega - \omega_0)^m]$, then we find

$$G_{\rm em} = \frac{32\pi e^2 a \Delta_{\downarrow}}{N|\Delta|SV_0} \exp[-1.024d\sqrt{V_0}] \left(N_{\downarrow}^L(0)N_{\uparrow}^R(0) + \frac{\Delta_{\downarrow}'}{\Delta_{\downarrow}}N_{\uparrow}^L(0)N_{\downarrow}^R(0) \right) \int_{\omega_c}^{V+k_BT} d\omega\omega^n \\ \times \exp[-b(\omega-\omega_0)^m] \left(1 + \frac{1}{\exp\left[\frac{\omega}{k_BT}\right] - 1} \right), \quad (63)$$

$$G_{\rm abs} = \frac{32\pi e^2 a \Delta_{\uparrow}}{N|\Delta|SV_0} \exp[-1.024d\sqrt{V_0}] \left(N_{\downarrow}^L(0)N_{\uparrow}^R(0) + \frac{\Delta_{\uparrow}'}{\Delta_{\uparrow}}N_{\uparrow}^L(0)N_{\downarrow}^R(0) \right) \int_{\omega_c}^{V+k_BT} d\omega\omega^n \\ \times \exp[-b(\omega-\omega_0)^m] \frac{1}{\exp\left[\frac{\omega}{k_BT}\right] - 1}. \quad (64)$$

The total conductance is simply given by $G=G_d+G_{em}$ + G_{abs} . For the sake of simplicity we make n=1 and m=2 in the magnon density of states (another possibility is to choose $n=1, m=1, \omega_0=0$) and this choic naturally includes a cutoff in the magnon spectrum. With the following definitions:

$$\Lambda_1(V) = \int_{\omega_c}^{V+k_BT} d\omega\omega \exp[-b(\omega-\omega_0)^2],$$
$$\Lambda_2(V) = \int_{\omega_c}^{V+k_BT} d\omega\omega \exp[-b(\omega-\omega_0)^2] \frac{1}{\exp\left[\frac{\omega}{k_BT}\right] - 1}$$

we obtain

$$\Lambda_{1}(V) = \frac{1}{2b} \{ e^{-b(\omega_{0} - \omega_{c})^{2}} - e^{-b(V + k_{B}T - \omega_{0})^{2}} + \sqrt{\pi b} \omega_{0} \operatorname{Erf}[\sqrt{b}(V + k_{B}T - \omega_{0})] + \operatorname{Erf}[\sqrt{b}(\omega_{0} - \omega_{c})] \}$$
(65)

and

$$\Lambda_{2}(V) = \frac{k_{B}T\sqrt{b\pi}}{2b} \exp\left[\frac{1}{4b(k_{B}T)^{2}} - \frac{\omega_{0}}{k_{B}T}\right]$$
$$\times \left(\operatorname{Erf}\left[\frac{1 + 2\sqrt{b}k_{B}T(V + k_{B}T - \omega_{0})}{2\sqrt{b}k_{B}T}\right]$$
$$- \operatorname{Erf}\left[\frac{1 + 2\sqrt{b}k_{B}T(\omega_{c} - \omega_{0})}{2\sqrt{b}k_{B}T}\right]\right), \tag{66}$$

where Erf(x) is the error function, defined below:

$$\operatorname{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp[-t^2/2] dt.$$

 $\Lambda_2(V)$ is zero for T = 0K meaning that absorption processes do not contribute to the current at extremely low temperatures. It is also convenient to define the expressions below

$$W_P^1 \approx |N_m^F|^2 \left(\frac{\Delta_{\perp}}{\Delta_{\uparrow}} + \frac{\Delta_{\perp}'}{\Delta_{\uparrow}}\right) r, \tag{67}$$

$$W_P^2 \approx |N_m^F|^2 \left(1 + \frac{\Delta_{\downarrow} + \Delta_{\uparrow}' + \Delta_{\downarrow}'}{\Delta_{\uparrow}}\right) r, \tag{68}$$

$$W_{\rm AP}^{\rm l} \approx |N_m^F|^2 \left(\frac{\Delta_{\downarrow}}{\Delta_{\uparrow}} + \frac{\Delta_{\downarrow}'}{\Delta_{\uparrow}} r^2 \right),$$
 (69)

$$W_{\rm AP}^2 \approx |N_m^F|^2 \left(1 + \frac{\Delta_{\downarrow}}{\Delta_{\uparrow}} + \frac{\Delta_{\uparrow}' + \Delta_{\downarrow}'}{\Delta_{\uparrow}}r^2\right).$$
(70)

Notice that the functions W_C^i defined above are related only to the density of states of the electrons in the electrodes. The desired result is

$$G_{\rm em}^{P} + G_{\rm abs}^{P} = \frac{32\pi e a \Delta_{\uparrow}}{N|\Delta|SV_{0}} \exp[-1.024d\sqrt{V_{0}}][W_{P}^{1}\Lambda_{1}(V) + W_{P}^{2}\Lambda_{2}(V)],$$
(71)

$$G_{\rm em}^{\rm AP} + G_{\rm abs}^{\rm AP} = \frac{32\pi e a \Delta_{\uparrow}}{N|\Delta|SV_0} \exp[-1.024d\sqrt{V_0}][W_{\rm AP}^1\Lambda_1(V) + W_{\rm AP}^2\Lambda_2(V)].$$
(72)

In Fig. 2 we show the resistance obtained with the formulas above, at T=0 K and at room temperature T=300 K. The experimental data was taken from Refs. 2, 3, and 10 and we have used in the theoretical calculations the following parameters: d=1.0 nm, $V_0=3.0$ eV, $N_m^F=1.0$ in normalized units, r=2.21, $\lambda=0.1$, $\beta=2.85$, and $\eta=0.1$. The parameter $2a\Delta_{\uparrow}/N|\Delta|S$ acts as T^J/T^d in the previous works^{10,19} and we have used $2a\Delta_{\uparrow}/N|\Delta|S=1/35$. The parameters appearing in the magnon spectrum are $\omega_0 = 16$ meV, $\omega_c = 4$ meV, and b = 500 eV^{-2} . The magnon density of states here is not of the form $\sqrt{\omega}$ as one would expect for surface magnons, however, the chosen spectral density eliminates the divergence at ω =0 coming from the Bose-Einstein distribution and the low cutoff frequency ω_c could be zero. The value of ω_0 agrees with the experimental data of the Ref. 1. We set functions W^i to be $W_P^1 = W_P^2/2 = 1.5 |N_m^F|^2 r$ and $W_{AP}^1 = W_{AP}^2/2 = |N_m^F|^2 (1.2)$ +1.7 r^2). It is considered that the direct current at T=0 K and T=300 K are the same (except for an offset $V \rightarrow V + k_B T$ at T=300 K), which means that we neglect temperature influences on the softening of the Fermi-Dirac distributions. The thermal effects enter only via the magnon processes. The exact temperature dependence depends on the magnon density of states. The factor $\Lambda_2(V)$ is the main responsible for the temperature dependence. In our model the temperature dependence is proportional to k_BT , though it varies according to the choice of the magnon spectrum. The MR decreases



FIG. 2. Resistance as a function of the voltage bias for the AP and *P* configurations: the experimental results (dotted lines) are taken from Refs. 2, 3, and 10 and the theoretical ones (solid lines) are calculated with our formulas, using the following parameters: d=1.0 nm, $V_0=3.0$ eV, $N_m^F=1.0$ in normalized units, r=2.21, $\lambda = 0.1$, $\beta=2.85$, and $\eta=0.1$, $2a\Delta_{\uparrow}/N|\Delta|S=1/35$, $\omega_0=16$ meV, $\omega_c=4$ meV, and b=500 eV⁻² eV. The resistances are given in arbitrary units, normalized to the peak value at zero bias.

with increasing temperature ($\Delta R/R = 25\%$ at T = 0 K and $\Delta R/R = 20\%$ at T=300 K), as one should expect, due to the fact that, for the AP alignment the resistance decays faster than for the P alignment. It is also a consequence of the magnon processes, which depends on the majority spin bands product $N_M^F N_M^F$ for AP configuration and on $N_m^F N_M^F$ for P. In Ref. 20 the existence of an inelastic spin-independent conductance is suggested (due to phonon excitation and barrier imperfections, for example) and the thermal effects in the Fermi-Dirac distributions seem to be important as proposed in Ref. 3. The behavior of a perfect MTJ is well explained mainly at low temperatures. The zero-bias anomaly tends to disappear with increasing temperature when the thermal effects on the Fermi-Dirac distributions is taken into account. The asymmetric behavior of the conductance with the bias voltage17 in practical MTJ's can be explained making the densities of states different from one electrode to another. The majority and minority spin bands may change from one electrode to another due to an impurity scattering center inside the barrier and/or imperfection and roughness of the interface surfaces. We have considered along this paper a simple band structure and we left the discussion of a realistic electronic structure of excited electrons as done in Ref. 21 in transition ferromagnetic metals aside.

V. CONCLUSIONS

In the present contribution we analyzed rigorously the spin-dependent transmission coefficients in a typical MTJ. The formulas obtained here agrees with both the intuition and the expressions used in Ref. 18 and allowed one to explore the main transport properties such as bias and temperature dependence of the conductance and MR in a perfect MTJ. We have presented a consistent study of the voltage

and temperature dependence of the "giant" magnetoresistance in ferromagnetic tunneling junctions. Our approach includes (a) a rigorous analysis of the spin-dependent transmission coefficients where conduction electrons were considered to be of s character and modeled by plane waves, interacting with spin wave excitations mainly at the interfaces between metallic ferromagnet and nonferromagnetic insulator. The electron-magnon interaction was considered as a perturbation. (b) Different variations of the density of states for each spin band with voltage. (c) Magnon assisted inelastic tunneling near zero bias, which enter via the transmission coefficients. We found that taking into account all those effects is essential to fully explain experimental results for the voltage range between 0 and 500 mV. Temperature effects are also taken into consideration. The role of the different parameters used in the theory was discussed in Ref. 19: some of them (d, Φ_0, η) determine the absolute value of the resistance at zero bias, which in turn is a scale factor in the theory; a different set, related to the band structure (r, β, λ) , mainly monitors the global behavior with voltage and the value of the junction MR. To adjust our results with selected experimental data, we have taken $\beta, \lambda > 0$, but as shown in Ref. 12, this scenario is not unique and depends on the topology of the bands that contribute to the current; and finally, the behavior near zero bias (zero bias anomaly), with a rapid decrease of the resistance for the AP configuration up to 100 mV, is ascribed to magnon-assisted tunneling. Our estimation of $2a\Delta_{\uparrow}/N|\Delta|S \approx T^{J}/T^{d} \sim 1/40$ seems to be more realistic than previous estimations.¹⁰ Our calculation is in excellent agreement with the experimental data (see Fig. 2).

Asymmetric behavior of the conductance with the bias voltage $[G(V) \neq G(-V)]$ can be ascribed to imperfections and roughness in the interface surfaces as well as to impurity inside the barrier.¹⁸ Another mechanism is a different coupling of majority and minority spin electrons to the spin waves as described in Ref. 17. However, our model explains the transport properties of a perfect ferromagnetic tunneling junction (perfect interfaces and no impurities inside the insulating barrier). The conductance asymmetries could be taken into account by making the densities of states different from one electrode to another.

Finally, the temperature effects have entered only via magnon scattering and the dependence is a function of the magnon spectrum. In Ref. 3 the thermal smearing in the Fermi-Dirac distribution of the tunneling electrons is analyzed and in Ref. 20 another inelastic mechanism which is spin independent is proposed to give an important contribution to the temperature dependence.

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