# Resonant spin-dependent tunneling in spin-valve junctions in the presence of paramagnetic impurities

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The tunnel magnetoresistance (TMR) of $F/O/F$ magnetic junctions ($F$'s are ferromagnetic layers and $O$ is an oxide spacer) in the presence of magnetic impurities within the barrier, is investigated. We assume that magnetic couplings exist both between the spin of the impurity and the bulk magnetization of the neighboring magnetic electrode, and between the spin of the impurity and the spin of the tunneling electron. Consequently, the resonant levels of the system formed by a tunneling electron and a paramagnetic impurity with spin $S=1$ are a sextet, and the resonant tunneling depends on the direction of the tunneling electron spin. At low temperatures and zero bias voltage, the TMR of the considered system may be larger than that of the same structure without paramagnetic impurities. It is calculated that an increase in temperature leads to a decrease in the TMR amplitude due to excitation of spin-flip processes resulting in mixing of spin-up and down channels. It is also shown that asymmetry in the location of the impurities within the barrier can lead to asymmetry in $I(V)$ characteristic of impurity-assisted current. Two mechanisms responsible for the origin of this effect are identified. The first one is due to the excitation of spin-flip processes at low voltages and the second one arises from the shift of resonant levels inside the insulator layer under high applied voltages.

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## I. INTRODUCTION

The observation of the large tunneling magnetoresistance effect at room temperature in tunnel junctions of the form $M/O/M'$ (where $M$ and $M'$ are magnetic metals and $O$ is an oxide tunnel barrier) has stimulated a renewed interest for these systems.[1–3] In addition to the fundamental interest for spin-polarized transport, these structures are also foreseen as potential candidates for sensitive magnetic sensors and memory cells in random access memory devices. The first model of spin-dependent tunneling in the framework of classical quantum mechanics was proposed by Słonczewski.[4] However, in this approach no scattering of electrons in the magnetic metallic electrodes was taken into account. This model has been subsequently developed in Refs. 5,6 by using the Kubo formalism of linear response. The effects of elastic impurity scattering inside the metallic layers and at interfaces between the dielectric and conductive layers could then be incorporated in the model. On the other hand, it is well known[7] that the presence of impurities inside the potential barrier can lead to the mechanism of resonant tunneling when the localized electronic states within the gap of the insulator formed by embedded atoms lie close to the chemical potential of the system. This situation was qualitatively studied in a mesoscopic semiconductor system[8] in the case of one- and two-impurity resonant channels by means of a classical quantum-mechanical treatment. The same approach has been used in Ref. 9 and applied to impurity-assisted tunneling magnetoresistance (TMR). The numerical analysis of this problem which was carried out in Refs. 10,11 should also be mentioned. In Ref. 9 only the case of spinless impurities was considered, and the author came to the conclusion that the TMR amplitude decreases due to impurity-assisted tunneling. The problem of paramagnetic impurity-assisted tunneling in tunnel magnetic junctions was investigated recently in Ref. 12, but two essential physical features have not been treated properly in this work. First, only one resonance channel, corresponding to the highest spin state of the impurity, has been considered as an additional contribution of impurity scattering to the tunnel current. The possible inelastic nature of such a spin-flip process has not been taken into account and as a result the so-called zero-bias anomaly is not traced in the obtained temperature dependence of magnetoresistance. Secondly, the linewidths of impurity levels have not been considered, but as it will be shown below they do depend on the position of the impurity atom inside the barrier as well as on the magnetic configuration of the magnetic layers. Moreover, these linewidths actually define the value of the tunneling conductance and the amplitude of the TMR for spin-conserving and spin-flip resonant tunneling. An attempt at an analysis of the same problem has also been undertaken in Refs. 13,14, but the microscopic mechanism of electron scattering on the paramagnetic impurity was also not taken into account.

In this paper, we propose a renewed study of the problem of impurity-assisted tunneling in spin-valve junctions of the form $F_1/O/F_3$, where $F$'s are ferromagnetic electrodes and $O$ is an insulating barrier with embedded paramagnetic impurities that incorporates the effect of both elastic and nonelastic spin-flip scattering due to the exchange interaction between the itinerant electrons forming the tunneling current and the localized spins of impurities. It will be shown that nonelastic scattering has an essential impact not only on the temperature variation of the TMR (which is a well-established result[15]) but also on the $I-V$ characteristics of the considered structures. The latter effect was predicted in Ref. 15, where the TMR dependence on the electron scattering by interfacial magnons was investigated.

 

## II. MODEL

### A. Kubo formula and general expression for the conductivity of the system

The following simplified model is adopted throughout the paper. First of all, the thickness of an oxide layer is supposed to be much smaller than its in-plane dimension and the interfaces are assumed to be flat, so that they may be considered as homogeneous in the $xy$ plane (parallel to the interfaces). We also denote the axis perpendicular to the $xy$ plane as the $z$ axis. Within each layer, the electrons are described as a free-electron gas and they undergo scattering on the three-dimensional (3D) $\delta$ function impurity potential within the insulating barrier. In the present article we have no intention of incorporating the features of the possible interfacial roughness as well, which always takes place and critically depends on the conditions of a preparation of the insulator layer. We only note that from a theoretical point of view, the influence of electron scattering at the metal/oxide interface due to interfacial roughness was investigated in our earlier work.[6] It was shown that two contributions to the tunnel current exist, one is due to a specular transmission through the barrier (ballistic conductance) and the other one is due to tunneling assisted by interfacial scattering (diffusive conductance). In the present article we focus our attention on the resonant impurity scattering and will not take into consideration the contribution of the diffusive conductance. Nevertheless, this in no way affects the qualitative conclusions made further in the text and if necessary, both mechanisms of interfacial and impurity-assisted scattering can be treated simultaneously. Thus, within these approximations, the Hamiltonian of the system has the form

$$\hat{H}=\hat{H}_0+\hat{H}_{\rm int},$$

where

$$\hat{H}_0=-\frac{\hbar^2}{2m(z)}\Delta+U(z)-2\mu_B H_z^{\rm eff}(z)(\hat{s}_z+\hat{S}_z^i)$$

$$\hat{H}_{\rm int}=\sum_i a_0^3\delta(\mathbf{r}-\mathbf{c}_i)\{\varepsilon_0-J(\mathbf{s}\mathbf{S}^i)\}. \tag{1}$$

Here the summation is performed over the location of impurities $\mathbf{c}_i$ inside the barrier, $a_0$ is the lattice constant, $\varepsilon_0$ denotes the scattering potential amplitude on the impurity, $J$ is the amplitude of the $s$-$d$-type exchange interaction between a conduction electron spin $\mathbf{s}$ and the impurity spin $\mathbf{S}^i$, $U(z)$ is a model steplike potential seen by the conduction electron as represented in Fig. 1. The potential profile is assumed to depend on the orientation of magnetizations of ferromagnetic layers. We take into account the exchange splitting of the $d$ band by introducing different values $V_\mu^{1,3}$ for the position of the bottom of the conduction band in $F_1$ and $F_3$, depending on the mutual orientation of magnetization in the layers and the spin $\mu=\uparrow,\downarrow$ of the conduction electron.

$H_z^{\rm eff}(z)$ represents the effective field acting on impurity and electron spins inside the barrier. The origin of this field is the superexchange between the spins in the bulk of ferromagnetic layer and in the insulating layer. We suppose that the impurity ion and a hopping electron form the intermediate resonance quantum state with the finite but long enough life-time and with total spin $(\mathbf{s}+\mathbf{S})$. It is possible due to the exchange interaction between the spin of electron and the spin of impurity, which is characterized by the parameter $J$. But in addition to this interaction, the weaker one exists between the total spin $(\mathbf{s}+\mathbf{S})$ and itinerant electrons in the bulk of ferromagnet which is included in the Hamiltonian (1) similar to the term proportional to $H^{\rm eff}(z)$. Since we suppose that impurity ions are located at the distance of the order of 2 atomic layers from the interface this interaction can be realized via atoms of oxygen (superexchange) and cannot be considered as negligibly small. We suppose that $H_z^{\rm eff}(z)$ decreases exponentially with the distance from the interface in the depth of the oxide layer. In the case when the embedded impurity ion has, e.g., spin $S=1$, the total system of resonant levels will form a multiplet: one doublet and one quartet.

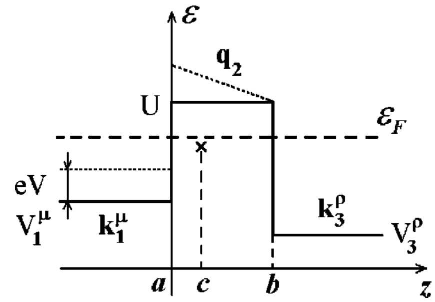


FIG. 1. The potential profile seen by electron propagating through the $F/O/F$ junction comprising impurity defect inside the oxide spacer. $k_1^\mu$, $k_3^\rho$, $q_2$ are the momenta inside the magnetic layers and oxide barrier, respectively. $V_{1(3)}^{\mu(\rho)}$ denotes the spin-dependent conduction band bottom, $U$ is a level of the barrier, and $\varepsilon_F$ is Fermi energy. The paramagnetic impurity is located at point $c$. The variation of the potential profile under high bias voltage is indicated by the dashed line.

Next, $m(z)$ corresponds to the effective electron mass that we suppose is equal to $m$ in the ferromagnetic layers and to $m_0$ in the insulator. Throughout the paper, it is expressed in units of bare electron mass $m_e$. We also assume that the mass of freelike electrons in the ferromagnet only slightly differs from $m_e$, i.e., $m\approx 1$ and we will eliminate it from all subsequent expressions.

We start from the Keldysh technique for Green functions together with Kubo exact formula of linear response theory for the static conductivity which relates its real part with the current-current correlation function and may be written in the form[16]

$$\sigma_{\mu\rho}(\mathbf{r},\mathbf{r}')=\frac{1}{2k_BT}\int_{-\infty}^{+\infty}\langle j_\rho(\mathbf{r}',t')j_\mu(\mathbf{r},t)\rangle d(t-t')$$
$$=\frac{1}{2k_BT}\left(\frac{e\hbar}{2m}\right)^2\int_{-\infty}^{+\infty}\langle G_{\mu\rho}^{<}(\mathbf{r},t,\mathbf{r}',t')\overleftrightarrow{\nabla}_{\mathbf{r}}\overleftrightarrow{\nabla}_{\mathbf{r}'}$$
$$\times G_{\rho\mu}^{>}(\mathbf{r}',t',\mathbf{r},t)\rangle d(t-t'), \tag{2}$$

where $\mu$, $\rho$ denote the projections of the spin of the electrons, $\overleftrightarrow{\nabla}_{\mathbf{r}}=(\vec{\nabla}_{\mathbf{r}}-\overleftarrow{\nabla}_{\mathbf{r}})$ is the asymmetric gradient operator, and $G^{<}_{\mu\rho}$ and $G^{>}_{\rho\mu}$ are corresponding Green functions in the Keldysh formalism.[17] $\langle\cdots\rangle$ represents the quantum statistical averaging over the distribution of impurities and degrees of freedom of the impurity spin. This expression is most general and holds both for the elastic impurity and defect scattering or inelastic, including magnon and phonon, scattering. Furthermore, in this work we restricted ourselves to the case of a low concentration of impurities and consider the regime of only one-channel resonant tunneling through the impurity levels. (For the case when the current may pass through channels with two resonant impurities see, e.g., Ref. 8.) In view of this, we calculated, first of all, the conductivity of an ''imaginary'' auxiliary system, comprising only one impurity located at the given point **c**. After this was done, averaging over distribution of impurities was performed in obtained expressions and the details of this averaging procedure are presented below in the text in Secs. II B and II C. To evaluate the conductivity (2) we exploit the perturbation theory by the impurity potential $H_{\rm int}$ in Eq. (1) with the use of the Keldysh diagrammatic technique. It may be effected rather straightforwardly if one knows the initial four-component Keldysh electron Green function of the unperturbed system (for more details see Appendix A). All these components can easily be expressed via the retarded Green function $G^{R}_{\mu\rho}$ corresponding to the Hamiltonian $H_0$. In our particular case it refers to the system which is homogeneous in the $xy$ plane and is inhomogeneous only in the $z$ direction. Therefore it can be found by solving the following differential equation:

$$\left\{\varepsilon+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}-\frac{\kappa^2}{2m}-U(z)\right\}G^{R}_{\mu\rho}(z,z',\kappa,\varepsilon)=\delta_{\mu\rho}\delta(z-z')$$

in the mixed real-space momentum representation,[5,6] where $\kappa=(\kappa_x,\kappa_y)$ is the component of the electron momentum in the $xy$ plane of the layers and $z$ is the coordinate perpendicular to the $xy$ plane. We should note that by definition the conductivity (2) is defined as a linear response on the externally applied electric field and does not depend on $z$ and $z'$ because of the obvious condition $\partial j(z)/\partial z=0$.

Let us now denote $k_1^{\mu}=\sqrt{2(\varepsilon-V_1^{\mu})}$, $k_3^{\mu}=\sqrt{2(\varepsilon-V_3^{\mu})}$ as the momenta of electrons with energy $\varepsilon$ and spin $\mu$ in the ferromagnetic layers and $q_0=\sqrt{2m_0(U-\varepsilon)}$, the imaginary momentum inside the barrier. By introducing the functions on $x=\kappa/q_0$

$$p_1^{\mu}(x)=\sqrt{k_1^{\mu 2}-q_0^2x^2},\quad p_3^{\mu}(x)=\sqrt{k_3^{\mu 2}-q_0^2x^2},$$

$$q_2(x)=q_0\sqrt{1+x^2},$$

the final expression for the conductance of the system, comprising only one impurity located at point **c**, at a given temperature $T$, is written as

$$\sigma(T,\mathbf{c})=\sigma_0(T)+\sigma^{\rm imp}(T,\mathbf{c}).$$

The first term is given by

$$\sigma_0(T)=\frac{q_0^2e^2}{2\pi\hbar}\sum_{\mu}\int_{-\infty}^{+\infty}d\varepsilon\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)\times\int_0^{x_0^{\mu}}\frac{x\,dx}{2\pi}\frac{16p_1^{\mu}p_3^{\mu}m_0^2q_2^2e^{-2q_2w}}{(m_0^2p_1^{\mu 2}+q_2^2)(m_0^2p_3^{\mu 2}+q_2^2)},\quad(3)$$

where $x_0^{\mu}=\min\{k_1^{\mu}/q_0,k_3^{\mu}/q_0\}$, $f(\varepsilon)=[1+e^{\beta(\varepsilon-\varepsilon_F)}]^{-1}$ is the Fermi function, and $w=b-a$ is the width of the insulating spacer. This represents the well-known result for the pure tunneling conductance.[4] The second term $\sigma^{\rm imp}(T,\mathbf{c})$ is directly related to the impurity assisted tunneling. It is convenient to write it down as a sum of two contributions

$$\sigma^{\rm imp}(T,\mathbf{c})=\sigma^{\rm imp}_{\rm el}(T,\mathbf{c})+\sigma^{\rm imp}_{\rm sf}(T,\mathbf{c}),$$

where the first term corresponds to the conductivity due to elastic spin-conserving processes of electron scattering at the impurity site and the second one summarizes all other events involving a change in the spin of the electron during the tunneling through the barrier. We have derived the analytical expressions for these two terms, which are valid under two assumptions: (i) domination of single electron scattering on impurities over multiple scattering of two and more electrons on the same center and (ii) absence of polarization of impurity spin induced by the ejection of spin-polarized electrons. Then the final result for these terms is written as (the details of its derivation are outlined further)

$$\sigma^{\rm imp}_{\rm el}(T,\mathbf{c})=\frac{1}{A}\left(\frac{2e^2}{\pi\hbar}\right)\int_{-\infty}^{+\infty}d\varepsilon\left\{-\frac{\partial f_{\uparrow}(\varepsilon-\mu_BH_z^{\rm eff})}{\partial\varepsilon}\times\langle(\hat{t}_z^{\uparrow}(\varepsilon))^{\dagger}\hat{t}_z^{\uparrow}(\varepsilon)\rangle\Phi^L_{\uparrow}(\mathbf{c})\Phi^R_{\uparrow}(\mathbf{c})-\frac{\partial f_{\downarrow}(\varepsilon+\mu_BH_z^{\rm eff})}{\partial\varepsilon}\times\langle(\hat{t}_z^{\downarrow}(\varepsilon))^{\dagger}\hat{t}_z^{\downarrow}(\varepsilon)\rangle\Phi^L_{\downarrow}(\mathbf{c})\Phi^R_{\downarrow}(\mathbf{c})\right\},\quad(4)$$

$$\sigma^{\rm imp}_{\rm sf}(T,\mathbf{c})=\frac{1}{A}\left(\frac{2e^2}{\pi\hbar}\right)\frac{1}{k_BT}\int_{-\infty}^{+\infty}d\varepsilon\{f_{\uparrow}(\varepsilon-\mu_BH_z^{\rm eff})\times[1-f_{\downarrow}(\varepsilon+\mu_BH_z^{\rm eff})]\langle\hat{t}_-(\varepsilon)\hat{t}_+(\varepsilon)\rangle+f_{\downarrow}(\varepsilon+\mu_BH_z^{\rm eff})[1-f_{\uparrow}(\varepsilon-\mu_BH_z^{\rm eff})]\times\langle\hat{t}_+(\varepsilon)\hat{t}_-(\varepsilon)\rangle\}\frac{1}{2}\{\Phi^L_{\uparrow}(\mathbf{c})\Phi^R_{\downarrow}(\mathbf{c})\times\Phi^L_{\downarrow}(\mathbf{c})\Phi^R_{\uparrow}(\mathbf{c})\}.$$

Here $A$ is the junction area, $\Phi^L_{\uparrow(\downarrow)}(\mathbf{c})$ and $\Phi^R_{\uparrow(\downarrow)}(\mathbf{c})$ are the probabilities of tunneling of the electron from the left or from the right electrode to impurity, located at point **c**. Omitting the exponentially small terms, the expression for these probabilities can be written as

$$\Phi^L_{\mu}(\mathbf{c})=\int_0^{x^{\mu}_{\rm max}}\frac{x\,dx}{2\pi}\frac{2p_1^{\mu}m_0^2q_0^2}{(m_0^2p_1^{\mu 2}+q_2^2)}e^{-2q_2(c-a)},$$

$$\Phi^R_\rho(\mathbf{c})=\int_0^{x^\rho_{\max}}\frac{x\,dx}{2\pi}\,\frac{2p^\rho_3 m_0^2 q_0^2}{(m_0^2 p_3^{\rho 2}+q_2^2)}e^{-2q_2(b-c)}.$$

The brackets $\langle\cdots\rangle$ in Eq. (4) denote thermodynamic averaging over degrees of freedom of the impurity spin and they imply the trace with the density matrix $\hat\rho_0=Z^{-1}\exp\{2\mu_B H_z^{\rm eff}\hat S_z/k_BT\}$, i.e., $\langle\hat t_\mu\hat t_\rho\rangle(\varepsilon)=\mathrm{Sp}\{\hat\rho_0\hat t_\mu(\varepsilon)\hat t_\rho(\varepsilon)\}$, $Z$ being the partition function. The quantities $\langle(\hat t_z^{\uparrow(\downarrow)})^\dagger\hat t_z^{\uparrow(\downarrow)}\rangle(\varepsilon)$ and $\langle\hat t_-\hat t_+\rangle(\varepsilon)$, $\langle\hat t_+\hat t_-\rangle(\varepsilon)$ in Eq. (4) represent the scattering amplitudes of electron on the impurity center for the case of spin conserving ($|\mathrm{in},\uparrow\rangle\to|\mathrm{out},\uparrow\rangle$) or $|\mathrm{in},\downarrow\rangle\to|\mathrm{out},\downarrow\rangle$) and spin-flip ($|\mathrm{in},\uparrow\rangle\to|\mathrm{out},\downarrow\rangle$ or $|\mathrm{in},\downarrow\rangle\to|\mathrm{out},\uparrow\rangle$) transitions averaged over the distribution of paramagnetic impurity spin. Here $|\mathrm{in}\rangle$ and $|\mathrm{out}\rangle$ denote the initial and final states of impurity. Operators $\hat t_z^{\uparrow(\downarrow)}$ and $\hat t_\pm$ are matrices acting in the subspace of impurity spin of a general dimension $(2S+1)$. They form a one-center scattering matrix

$$\hat t=\begin{pmatrix}\hat t_z^\uparrow & \hat t_-\\ \hat t_+ & \hat t_z^\downarrow\end{pmatrix}$$

in the direct product of the linear subspaces of electron's and impurity's spins and are expressed as

$$\hat t_z^{\uparrow(\downarrow)}(\varepsilon)=\frac{1}{1-\hat V_z^{\uparrow(\downarrow)}(\varepsilon)G_{\uparrow(\downarrow)}(\varepsilon)}\hat V_z^{\uparrow(\downarrow)}(\varepsilon),$$

$$\hat t_\pm(\varepsilon)=-\frac{1}{1-\hat V_z^{\downarrow(\uparrow)}(\varepsilon)G_{\downarrow(\uparrow)}(\varepsilon)}\hat S_\pm\times\frac{a_0^3 J/2}{1-a_0^3\left(\varepsilon_0+\frac{1}{2}J\hat S_z\right)G_{\uparrow(\downarrow)}(\varepsilon)},\qquad(5)$$

where effective potentials $\hat V_z^{\uparrow(\downarrow)}$ are given by

$$\hat V_z^{\uparrow(\downarrow)}(\varepsilon)=a_0^3\left\{\varepsilon_0\mp\frac{1}{2}J\hat S_z+\frac{1}{4}\hat S_\mp\frac{a_0^3G_{\downarrow(\uparrow)}(\varepsilon)J^2}{1-a_0^3\left(\varepsilon_0\pm\frac{1}{2}J\hat S_z\right)G_{\downarrow(\uparrow)}(\varepsilon)}\hat S_\pm\right\}.$$

These expression are general for an arbitrary spin number $S$ of the impurity, but further in this work we examined in details only the case of $S=1$. Then matrices $\hat t$ are reduced to the dimension $(3\times3)$ and the partition function $Z=2\cosh(2\mu_B H_z^{\rm eff}/k_BT)+1$. In Eq. (5) $G_{\uparrow(\downarrow)}(\varepsilon)$ denote the electron Green function at point $\mathbf{c}$:

$$G_\mu(\varepsilon,\mathbf{c})=\int_0^{\kappa_{\max}}G_{\mu\kappa}(\varepsilon,\mathbf{c})\frac{\kappa\,d\kappa}{2\pi},$$

where $\kappa_{\max}=2\sqrt{\pi}/a_0$ is a cutoff of in-plane momentum that stems from the finite size of Brillouin zone [we substitute the projection of the Brillouin zone onto the $(\kappa_x,\kappa_y)$ plane by the circle of radius $\kappa_{\max}$ of the same square in the $\kappa_\parallel$ plane]. The real and imaginary part of $G^\mu_\kappa(\varepsilon,\mathbf{c})$ ($\mu$ is the spin index) in the leading order of magnitude are given by

$$\mathrm{Re}\,G^\mu_\kappa(\varepsilon,\mathbf{c})=-\frac{m_0}{q_2},$$

$$\mathrm{Im}\,G^\mu_\kappa(\varepsilon,\mathbf{c})=-[\Phi^L_\mu(\mathbf{c})+\Phi^R_\mu(\mathbf{c})].\qquad(6)$$

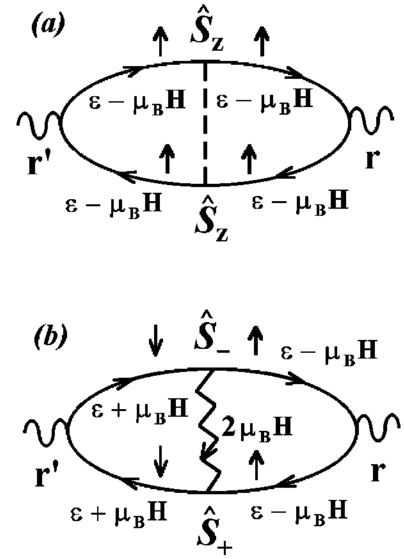


FIG. 2. Two diagrams that make contribution to the conductivity in the second order of the perturbation theory. Here the full lines correspond to the electron Green functions and wavy lines denote the asymmetric gradient operator of the velocity $\overleftrightarrow{\nabla}_{\mathbf{r}}$ with respect to sites $\mathbf{r}$ and $\mathbf{r}'$ of the diagram. The dashed and zig-zag lines represent the equilibrium spin-spin correlation functions. The former one correspond to the elastic spin-conserving process (a) and the latter to the nonelastic spin-flip process (b). (See details in Appendix A.)

Let us now explain the derivation of expression (4) and clarify the two assumptions under which this formula is valid. To derive (4) from the starting point (2) one can first of all examine two diagrams (a) and (b) (see Fig. 2) that contribute to the spin-conserving and spin-flip parts of $\sigma^{\rm imp}(T,\mathbf{c})$ at second order of $J$, respectively. One may easily verify that the general structure of these diagrams is the same as the final result in form (4) with the mere difference that the one-center $t$ matrix is reduced at first order of $J$ to the initial potential

$$\varepsilon_0-(J/2)\begin{pmatrix}\hat S_z & \hat S_-\\ \hat S_+ & -\hat S_z\end{pmatrix}.$$

Moreover, diagram (b) contains both direct and indirect processes in equal proportion with common factor 1/2 for any of the possible channels $|\mathrm{in},\uparrow\rangle\to|\mathrm{out},\downarrow\rangle$ or $|\mathrm{in},\downarrow\rangle\to|\mathrm{out},\uparrow\rangle$. The thermodynamic averaging $\langle\cdots\rangle$ in the second-order expansion is simply reduced to the averaging over the Boltzman distribution of the impurity spin in the ''external'' effective magnetic field $H_z^{\rm eff}$ which was introduced in Eq. (1), i.e., with the density matrix $\hat\rho_0$ as it was described above in the text. After that, it is easy to check that the total probabilities (with account taken of Fermi factors of electron states) of direct and inverse processes are equal which means that the principle of detailed equilibrium holds. In particular it leads to the vanishing of spin-flip processes in a system at zero temperature and vanishing voltage bias.

After that preliminary discussion two assumptions must be made to justify the result (4).

(i) We assume that the occupation electrons rare event thus we exclude the double occupancy at an impurity site in our model. It may be justified by (a) the strong Coulomb electron-electron interaction that make unprofitable their arrangement at the same site of a lattice and (b) the large number of impurity centers that provides a sufficiently large number of one-step channels.

(ii) We also neglect the influence of the electron current on the statistical distribution of paramagnetic spins inside the oxide barrier. This assumption is valid for a practical intensity of tunneling current which is low enough not to produce a spin polarization of impurities by the injection of spin-polarized charge carriers. So we will consider the case of a small deviation of the electron's distribution function from its equilibrium value. However, even for that case it is justifiable to calculate the nonlinear *I-V* characteristic in the way done in Sec. II D [see Eq. (17)].

Under these assumptions, expression (4) can be obtained by a simple substitution of the scattering potential $\hat{H}_{\rm int}$ at the site $\mathbf{c}_i$ in Fig. 2 by the corresponding one-center *t* matrix in accordance with Eq. (5) and assuming that averaging over the degrees of freedoms of the impurity is carried out by means of the unperturbed density matrix $\hat{\rho}_0 = Z^{-1}\exp\{2\mu_B H_z^{\rm eff}\hat{S}_z/k_BT\}$. In this form, the structure of the result (4) is similar to the one obtained in Ref. 15, where the spin-flip scattering of electrons at interfaces of tunnel junctions was investigated in the framework of a tunneling Hamiltonian and the second order perturbation theory.

### B. Resonant tunneling in the case of nonmagnetic impurities

To extract the physical nature of resonant tunneling through the impurity states contained in expression (4), we proceed as follows. For the sake of clarity and simplicity we consider first the case of zero-spin impurity. Then only one element of *t* matrix at site $\mathbf{c}$ remains

$$t_0^{\uparrow(\downarrow)}(\varepsilon) = \frac{a_0^3\varepsilon_0}{1-a_0^3\varepsilon_0 G_{\uparrow(\downarrow)}(\varepsilon)}.$$

It defines the position of a resonant level inside the gap of the dielectric band structure by finding the root of the equation $a_0^3\varepsilon_0 {\rm Re}G_{\uparrow(\downarrow)}(\varepsilon_i)=1$. From expression (6), it follows that the real part of the Green function ${\rm Re}\,G_\mu(\varepsilon,\mathbf{c})$ is independent of $\mathbf{c}$ and spin $\mu$ up to exponentially small terms. Therefore, the position of level $\varepsilon_i$ is weakly dependent both on the position of impurity inside the barrier and on the direction of the spin of the tunneling electron. Evidently, only those impurities for which $\varepsilon_i$ is close to the chemical potential $\varepsilon_F$ contribute to a significant extent to the total current at low bias voltage. Therefore, it is possible to expand the denominator in $t_0^{\uparrow(\downarrow)}(\varepsilon)$ in powers of $(\varepsilon_i-\varepsilon)$. If we now introduce the position-dependent linewidths

$$\Gamma_\mu^L(\mathbf{c}) = \Phi_\mu^L(\mathbf{c})/{\rm Re}\,G'(\varepsilon_F), \quad \Gamma_\mu^R(\mathbf{c}) = \Phi_\mu^R(\mathbf{c})/{\rm Re}\,G'(\varepsilon_F), \tag{7}$$

where ${\rm Re}\,G'(\varepsilon_F) = (\partial/\partial\varepsilon){\rm Re}\,G(\varepsilon)|_{\varepsilon=\varepsilon_F}$ is the energy derivative of the electron Green function at the Fermi level, then we obtain the general formula for the resonant case of impurity assisted tunneling

$$\sigma^{\rm imp}(\mathbf{c}) \simeq \frac{2e^2}{\pi\hbar A}\int_{-\infty}^{+\infty}\sum_{\mu,i}\frac{\Gamma_\mu^L(\mathbf{c})\Gamma_\mu^R(\mathbf{c})}{(\varepsilon_F-\varepsilon_i)^2+\Gamma_\mu^2(\mathbf{c})}\left(-\frac{\partial f}{\partial\varepsilon}\right)d\varepsilon, \tag{8}$$

where $\Gamma_\mu(\mathbf{c}) = \Gamma_\mu^L(\mathbf{c}) + \Gamma_\mu^R(\mathbf{c})$, *A* is a junction area, and the summation on *i* is performed over all resonant levels. For the qualitative analysis, one may evaluate expressions (7) for $\Gamma_\mu^{R(L)}(\mathbf{c})$ approximately by considering the case $\kappa=0$ which is valid if $e^{-2q_0w}\ll 1$. In this approximation

$$\Gamma_\mu^L(\mathbf{c}) = \frac{2k_{1\mu}^F m_0}{m_0^2 k_{1\mu}^{F2}+q_0^2}\left(\frac{q_0^2}{2m_0}\right)\frac{e^{-2q_0(c-a)}}{c-a},$$

$$\Gamma_\mu^R(\mathbf{c}) = \frac{2k_{3\mu}^F m_0}{m_0^2 k_{3\mu}^{F2}+q_0^2}\left(\frac{q_0^2}{2m_0}\right)\frac{e^{-2q_0(b-c)}}{b-c}, \tag{9}$$

and expression (8) reproduces the result of Ref. 8. To proceed further, we discuss some assumptions concerning the parameters of the model. We consider the case of Co electrodes and $Al_2O_3$ as the tunnel barrier and take typical values of $k_\uparrow^F = 1.09$ Å$^{-1}$, $k_\downarrow^F = 0.42$ Å$^{-1}$, $m\approx 1$ for itinerant electrons in Co and a typical barrier height for $Al_2O_3$ (measured from the Fermi level $\varepsilon_F$) $U_0-\varepsilon_F = 3$ eV with an effective mass $m_0=0.4$ (Ref. 9), that gives $q_0\simeq 0.56$ Å$^{-1}$. Assuming the thickness of the barrier $w\simeq 20$ Å, one may estimate the conductance $\sigma_0$ of the system without impurity from Eq. (3) by means of the approximate formula

$$\sigma_0 \simeq \frac{2e^2}{\pi^2\hbar}\left(\frac{q_0}{w}\right)\sum_\mu \frac{k_{1\mu}^F k_{3\mu}^F q_0^2 m_0^2 e^{-2q_0w}}{(m_0^2k_{1\mu}^{F2}+q_0^2)(m_0^2k_{3\mu}^{F2}+q_0^2)}, \tag{10}$$

which leads to TMR≃16%. To estimate the value of the linewidth (9) we consider impurities located close to the left interface at a distance of, say, two atomic layers which corresponds to $(c-a)\simeq 4$ Å. For spin up electrons, this gives $\Gamma_\uparrow(\mathbf{c})\simeq 0.02$ eV. Further in this paper we restrict ourselves to the case of temperature interval from 4.2−300 K (0.025 eV). We assume that the impurity levels $\varepsilon_i$ in the band gap of the insulator form a narrow impurity band of width $\Delta\varepsilon$ which spreads symmetrically with respect to Fermi level $\varepsilon_F$. Furthermore, following Ref. 8, we introduce its density of states $\nu(\varepsilon)$ per unit area and unit energy interval. We assume that $\Delta\varepsilon$ is of the order of 0.1 to 0.2 eV, i.e., an order of magnitude greater that the above estimated linewidth. In this context, with a good accuracy, the impurity conductance (8) can be rewritten as

$$\sigma^{\text{imp}}(\mathbf{c}) \simeq \frac{2e^2\nu(\varepsilon_F)}{\hbar}\sum_{\mu}\int_{-\infty}^{+\infty}\left(-\frac{\partial f}{\partial \varepsilon}\right) \times \frac{\Gamma_\mu^L(\mathbf{c})\Gamma_\mu^R(\mathbf{c})}{\Gamma_\mu(\mathbf{c})}\rho(\varepsilon,\mathbf{c})d\varepsilon, \tag{11}$$

where the factor

$$\rho(\varepsilon,\mathbf{c}) = \frac{2}{\pi}\arctan\left(\frac{\Delta\varepsilon}{2\Gamma_\mu(\mathbf{c})}\right)$$

arises from the integration of Eq. (8) over impurity levels $\varepsilon_i$ in the range of impurity band. Due to the abovementioned estimations, equality $\rho(\varepsilon,\mathbf{c}) \simeq 1$ holds with a good degree of accuracy. In this case Eq. (11) is in agreement with Refs. 8,9.

### C. Resonant tunneling in the case of paramagnetic impurities

To investigate the general case of paramagnetic impurity, we follow the same procedure as in the previous section. Let $\mathbf{J}=\mathbf{s}+\mathbf{S}$ be the total magnetic moment of the system. We may state that $[H,J_z]=0$ and, therefore, $J_z$ is a good quantum number. We regard the $\hat{t}$ matrix (5) as an operator acting on the spinor subspace $|\sigma,m\rangle$, where $\sigma=\pm\frac{1}{2}$ and $m=\pm 1,0$ correspond to the projection of the $z$ component of the electron and impurity spin, respectively (we consider the case $\mathbf{S}=1$). As long as its total magnetic moment along the $z$ axis $J_z=s_z+S_z$ is conserved, the matrix elements $\langle\sigma_1 m_1|\hat{t}|\sigma_2 m_2\rangle$ are nonzero only if $m_1+\sigma_1=m_2+\sigma_2$. Therefore, it is convenient to introduce the notation $t_{m_j}^{\sigma_1\sigma_2}=\langle\sigma_1 m_1|\hat{t}|\sigma_2 m_2\rangle$, where $m_j=m_1+\sigma_1=m_2+\sigma_2$. These elements are simply calculated from Eq. (5). The nonzero ones are written as

$$t_{3/2}^{\uparrow\uparrow} = \frac{a_0^3(\varepsilon_0 - J/2)}{1-a_0^3(\varepsilon_0-J/2)G_\uparrow(\varepsilon)},$$

$$t_{-3/2}^{\downarrow\downarrow} = \frac{a_0^3(\varepsilon_0 - J/2)}{1-a_0^3(\varepsilon_0-J/2)G_\downarrow(\varepsilon)}, \tag{12}$$

and

$$\hat{t}_{\pm 1/2} = \begin{pmatrix} t_{\pm 1/2}^{\uparrow\uparrow} & t_{\pm 1/2}^{\downarrow\uparrow} \\ t_{\pm 1/2}^{\uparrow\downarrow} & t_{\pm 1/2}^{\uparrow\uparrow} \end{pmatrix}$$

corresponding to the subspace $m_j=\pm\frac{1}{2}$ with

$$t_{1/2}^{\downarrow\downarrow}(t_{-1/2}^{\uparrow\uparrow}) = \frac{a_0^3}{\Delta_{\pm 1/2}(\varepsilon)}\{\varepsilon_0 + J/2 - a_0^3 G_{\uparrow(\downarrow)}(\varepsilon)(\varepsilon_0 - J/2)(\varepsilon_0+J)\},$$

$$t_{1/2}^{\uparrow\uparrow}(t_{-1/2}^{\downarrow\downarrow}) = \frac{a_0^3}{\Delta_{\pm 1/2}(\varepsilon)}\{\varepsilon_0 - a_0^3 G_{\downarrow(\uparrow)}(\varepsilon)(\varepsilon_0-J/2)(\varepsilon_0+J)\},$$

$$t_{\pm 1/2}^{\uparrow\downarrow} = t_{\pm 1/2}^{\downarrow\uparrow} = -\frac{a_0^3}{\sqrt{2}\Delta_{\pm 1/2}}J, \tag{13}$$

where the denominators are

$$\Delta_{\pm 1/2}(\varepsilon) = [1-a_0^3 G_\downarrow(\varepsilon)(\varepsilon_0 - J/2)][1-a_0^3 G_\uparrow(\varepsilon)(\varepsilon_0+J)] \pm a_0^3 J[G_\uparrow(\varepsilon)-G_\downarrow(\varepsilon)].$$

As can be seen, two poles of the $\hat{t}$ matrix defined from equations $a_0^3 \mathrm{Re}\, G(\varepsilon_{3/2})(\varepsilon_0 - J/2)=1$ and $a_0^3 \mathrm{Re}\, G(\varepsilon_{1/2})(\varepsilon_0+J)=1$ correspond to two multiplets $\varepsilon_{3/2}$ and $\varepsilon_{1/2}$ with a total angular momentum $j=3/2$ and $j=1/2$, respectively. If $J>0$, then $\varepsilon_{3/2}<\varepsilon_{1/2}$, i.e., the multiplet with $j=3/2$ has a lower energy than the one with $j=1/2$. As for nonmagnetic impurity, we restrict ourselves by considering the regime of only one-channel resonant tunneling. We assume that $J>0$ and the lowest impurity levels $\varepsilon_i=\varepsilon_{3/2}$ corresponding to the multiplet with $j=3/2$ lie close to $\varepsilon_F$. We note that the typical value of exchange coupling $J$ is of order 1 eV and due to this fact we may eliminate the resonant level $\varepsilon_{1/2}$ from further consideration. Then, as in the previous analysis for a nonmagnetic impurity, only the resonant part of the $\hat{t}$ matrix (12), (13) at energies close to chosen $\varepsilon_{3/2}$ is essential for the subsequent calculations. Expressions (12), (13) can be easily written as

$$t_{\pm 3/2}^{\uparrow\uparrow(\downarrow\downarrow)}(\varepsilon) = \frac{1}{G'(\varepsilon)}\,\frac{1}{\varepsilon-\varepsilon_i+i\Gamma_{\uparrow(\downarrow)}(\mathbf{c})},$$

$$\hat{t}_{1/2}(\varepsilon) = \frac{1}{G'(\varepsilon)}\,\frac{1}{\varepsilon-\varepsilon_i+i\gamma_\uparrow(\mathbf{c})}\begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{2}{3}\end{pmatrix},$$

$$\hat{t}_{-1/2}(\varepsilon) = \frac{1}{G'(\varepsilon)}\,\frac{1}{\varepsilon-\varepsilon_i+i\gamma_\downarrow(\mathbf{c})}\begin{pmatrix} \frac{2}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{1}{3}\end{pmatrix}, \tag{14}$$

where $\gamma_\uparrow(\mathbf{c})=\frac{2}{3}\Gamma_\uparrow(\mathbf{c})+\frac{1}{3}\Gamma_\downarrow(\mathbf{c})$, $\gamma_\downarrow(\mathbf{c})=\frac{1}{3}\Gamma_\uparrow(\mathbf{c})+\frac{2}{3}\Gamma_\downarrow(\mathbf{c})$ are the inverse lifetimes of the resonant states with $m_j=\pm 1/2$. This result allows simple qualitative interpretation. Let us look, for example, at quantum states with $m_j=1/2$. From elementary quantum-mechanical theory, one may conclude that

$$\phi_{1/2}^{\uparrow} = |\uparrow, m_s=0\rangle = \sqrt{\frac{2}{3}}\left|j=\frac{3}{2},m_j=\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|j=\frac{1}{2},m_j=\frac{1}{2}\right\rangle,$$

$$\phi_{1/2}^{\downarrow} = |\downarrow, m_s=1\rangle = \sqrt{\frac{1}{3}}\left|j=\frac{3}{2},m_j=\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|j=\frac{1}{2},m_j=\frac{1}{2}\right\rangle. \tag{15}$$

As we have assumed, only $|j=\frac{3}{2},m_j=\frac{1}{2}\rangle$ gets into resonance and, therefore, e.g., $t_{1/2}^{\uparrow\downarrow}\sim\langle\phi_{1/2}^{\uparrow}|\hat{t}|\phi_{1/2}^{\downarrow}\rangle\sim\sqrt{2}/3$ in agreement with Eq. (14). On the other hand,

$$\left| j=\frac{3}{2},m_j=\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}|\uparrow,m_s=0\rangle + \sqrt{\frac{1}{3}}|\downarrow,m_s=1\rangle$$

and, hence, its inverse lifetime is given by $\tau_{1/2}^{-1}=\frac{2}{3}\tau_{\uparrow}^{-1}+\frac{1}{3}\tau_{\downarrow}^{-1}$.

We substitute all $\hat{t}$-matrix elements in Eq. (4) by its resonance expansion (14). To proceed further, one has to perform in Eq. (4) the configuration averaging over all impurity centers and thermodynamic one over all possible channels. Suppose, that the impurities are distributed uniformly in the space in the interval $[z_0-\Delta,z_0+\Delta]$ along the $z$ direction with the width of $2\Delta$ and center $z_0$ which we have chosen to be close to left ($L$) ferromagnetic contact. After that, it is possible, first of all, to average the Lorentzian peaks over the distribution of impurity levels by averaging them over $\varepsilon_i$ in the range of impurity band with factor $\nu(\varepsilon_F)$ and to perform the thermodynamic averaging by integrating over $\varepsilon$ and neglecting the dependencies of $\Gamma^{L(R)}(\mathbf{c})$ on energy. On the third step, the averaging over the space distribution of impurities along the $z$ direction should be made. Following the outlined procedure, the total conductance (4) as a function of temperature is written as a sum of factorized terms over all possible scattering channels

$$\sigma(T)=\frac{2e^2}{\hbar}\sum_{\mu\rho\, m_j} P_{m_j}^{\mu\rho}\left(\frac{\mu_B H_z^{\text{eff}}}{k_B T}\right)\sigma_{m_j}^{\mu\rho}(z_0,\Delta)\,\nu(\varepsilon_F)+\sigma_0, \tag{16}$$

where

$$\sigma_{m_j}^{\mu\rho}(z_0,\Delta)=\frac{1}{2\Delta}\int_{z_0-\Delta}^{z_0+\Delta}\sigma_{m_j}^{\mu\rho}(c)\rho(\varepsilon_F,c)dc.$$

The origin of $\rho(\varepsilon_F,c)$ is the same as in Eq. (11) and the explicit form of functions $P_{m_j}^{\mu\rho}(h)$ and $\sigma_{m_j}^{\mu\rho}(c)$ for parallel and antiparallel alignments of magnetization of the ferromagnetic layers is given in Appendix B. We have also used the same notation of matrix indexes as was previously introduced for $\hat{t}$-matrix elements. $\sigma_0$ is the tunnel conductance of the pure system in accordance with Eq. (3). Factors $P_{m_j}^{\mu\rho}$ and $\sigma_{m_j}^{\mu\rho}$ represent the thermodynamic and quantum-mechanical probabilities of the given process, respectively. Expressions (16) are the final results of this section and their analysis is presented below (see Sec. III).

### D. Dependence of conductivity on bias-voltage

We are also interested in the $I(V)$ characteristics of the considered system. To derive the general formula for the current, one may simply extend expressions (4) to the case of finite applied bias voltage. Consider, for example, the contribution to the total current $I$, coming from all possible channels of the form $|\text{in},\uparrow\rangle\rightarrow|\text{out},\downarrow\rangle$ for tunnel electrons moving from the left electrode to the right electrode and of the form $|\text{in},\downarrow\rangle\rightarrow|\text{out},\uparrow\rangle$ for electrons moving from right to left, respectively, i.e., in both cases an electron has an ''up'' projection of spin in the left contact and a ''down'' projection of spin in the right one after or before scattering. From this general concept, one may conclude that this contribution to the current can be written as

$$\begin{aligned} I^{\uparrow\downarrow}(V)=&\frac{1}{S}\left(\frac{2e^2}{\pi\hbar}\right)\int_{-\infty}^{+\infty}d\varepsilon\,\Phi_{\uparrow}^{L}(\mathbf{c})\Phi_{\downarrow}^{R}(\mathbf{c})\{\langle\hat{t}_-(\varepsilon)\hat{t}_+(\varepsilon)\rangle\\ &\times\{f_{\uparrow}(\varepsilon-\mu_B H_z^{\text{eff}}-eV)[1-f_{\downarrow}(\varepsilon+\mu_B H_z^{\text{eff}})]\\ &-\langle\hat{t}_+(\varepsilon)\hat{t}_-(\varepsilon)\rangle f_{\downarrow}(\varepsilon+\mu_B H_z^{\text{eff}})\\ &\times[1-f_{\uparrow}(\varepsilon-\mu_B H_z^{\text{eff}}-eV)]\}, \end{aligned} \tag{17}$$

where it is assumed that the voltage bias is applied from the left to right direction. It is important to notice that inelastic spin-flip processes of the electron scattering on the impurity were taken into account in derivation of the Eq. (17) but they were omitted in Ref. 12. Analogous expressions can be written for all other channels. In the case under consideration, expression (17) contains two regimes of nonlinear behavior of the $I(V)$ characteristic. The first one reproduces a zero bias anomaly due to excitation of spin-flip processes at low bias voltages of order of magnitude $\mu_B H_z^{\text{eff}}$ (we believe that it is of order 5 mV). In this range, as before, one may assume that the resonance amplitudes $\langle(\hat{t}_z^{\uparrow(\downarrow)})^{\dagger}(\hat{t}_z^{\uparrow(\downarrow)})\rangle$ and $\langle\hat{t}_-\hat{t}_+\rangle$ are nearly independent of the energy after averaging over all possible configurations of impurities. As a result, the voltage dependence of total current are given by formulas similar to Eq. (16):

$$I(V,T)=\frac{2e}{\hbar}\sum_{\mu\rho m_j} I_{m_j}^{\mu\rho}(V,H_z^{\text{eff}})\sigma_{m_j}^{\mu\rho}(z_0,\Delta)\,\nu(\varepsilon_F)+\sigma_0 V. \tag{18}$$

The expressions for $I_{m_j}^{\mu\rho}(V,H_z^{\text{eff}})$ for parallel and antiparallel configurations are given in Appendix C. The voltage dependent conductance $\sigma(V,T)$ can be obtained from Eq. (17) by derivation with respect to $V$. The detailed analysis of this physical situation is presented in the next section.

The second source of the possible nonlinear character of $I(V)$ dependence is the variation of potential profile $U(z)$ (see Fig. 1) under applied bias voltage. The latter indeed introduces corrections to Eqs. (9) and (10) which can be calculated with the use of Wentzel-Kramers-Brillouin (WKB) approximation,[18] assuming that the applied voltage produces a uniform electrical field inside the insulating layer. In the case of pure tunnel conductance, it is known[19] that both conductances for parallel and antiparallel configurations increase with the increasing applied voltage so that the TMR as a function of $V$, defined as $[I^P(V)-I^{AP}(V)]/I^{AP}(V)$, drops significantly at voltages of order 1 eV. The contribution of impurity assisted tunneling may change considerably this situation in the case of the nonuniform spatial distribution of impurities, e.g., when they are distributed in the vicinity of only one electrode. In this particular situation, as we will show, the essential variation of TMR amplitude in the case of magnetic impurities (in contrast to nonmagnetic ones) takes place at bias voltages comparable with impurity band width $\Delta\varepsilon$.

For the sake of simplicity, we consider, first, the case of non-magnetic impurities. In the WKB approximation, the contribution from all impurities, located at given point $\mathbf{c}$, to the total current $I(V)$ has a form similar to (9) and Eqs. (11):

$$j^{\mathrm{imp}}(\mathbf{c})=\frac{2e^2}{\hbar}\nu(\varepsilon_F)\sum_{\mu}\int_{-\infty}^{+\infty}d\varepsilon\{f(\varepsilon-eV)-f(\varepsilon)\}\times\frac{\Gamma_{\mu}^{L}(\mathbf{c})\Gamma_{\mu}^{R}(\mathbf{c})}{\Gamma_{\mu}^{L}(\mathbf{c})+\Gamma_{\mu}^{R}(\mathbf{c})}\rho(\varepsilon,V), \tag{19}$$

where

$$\Gamma_{\mu}^{L}(\mathbf{c})=\frac{k_{1\mu}^{F}q_a m_0\tau_a^{-1}}{(q_a^{-})^2+k_{1\mu}^{F2}m_0^2}e^{-S_a/\hbar};$$

$$\Gamma_{\mu}^{R}(\mathbf{c})=\frac{k_{3\mu}^{F}q_b m_0\tau_b^{-1}}{(q_b^{+})^2+k_{3\mu}^{F2}m_0^2}e^{-S_b/\hbar}. \tag{20}$$

Here $q_b^2=q_0^2=2m_0(U-\varepsilon)$, $q_a^2=q_0^2+2m_0\,eV$ are imaginary momenta of electron with energy $\varepsilon$ in the vicinity of the right and left electrodes, $q_{a(b)}^{\pm}=q_0\pm\frac{1}{2}(eEm_0/q_{a(b)}^2)$, $E$ is the electric field in the barrier. We also introduce $q_c=q_0+2m_0\,eV(b-c)/w$, the imaginary momentum of electron on the impurity center. Then $S_a=(q_a^3-q_c^3)/3m_0eE$, $S_b=(q_c^3-q_b^3)/3m_0eE$ represent the classical actions along the path from the left contact to the point $\mathbf{c}$ in the barrier and, afterwards, from this point to the right contact, respectively, $\tau_a=(q_a-q_c)/eE$ and $\tau_b=(q_c-q_b)/eE$ denote the passage times associated with these paths. The factor

$$\rho(\varepsilon,V)=\frac{1}{\pi}\left\{\arctan\left[\frac{\varepsilon-\varepsilon_F-eV\left(\frac{b-c}{w}\right)+\frac{\Delta\varepsilon}{2}}{\Gamma_{\mu}^{L}(\mathbf{c})+\Gamma_{\mu}^{R}(\mathbf{c})}\right]-\arctan\left[\frac{\varepsilon-\varepsilon_F-eV\left(\frac{b-c}{w}\right)-\frac{\Delta\varepsilon}{2}}{\Gamma_{\mu}^{L}(\mathbf{c})+\Gamma_{\mu}^{R}(\mathbf{c})}\right]\right\}, \tag{21}$$

as before, arises from the summation over all impurity levels $\varepsilon_i$ and gives the relative weight of all resonant channels with energy $\varepsilon$. To clarify the situation, it is sufficient to consider the most resonant channel with energy $\varepsilon_r=\varepsilon_F+eV(b-c)/w$ at which $\rho(\varepsilon,V)$ reaches its maximum. One may note that $\varepsilon_r$ corresponds to the resonant impurity level that exactly coincides with Fermi energy at vanishing voltage and it shifts linearly with the increase of applied bias depending on the position $\mathbf{c}$ of impurity inside the barrier. As stated earlier, the most interesting case takes place when the point $\mathbf{c}$ is situated close to the left contact. Then one can see that $\Gamma^{L}(\mathbf{c})\gg\Gamma^{R}(\mathbf{c})$ and, thus, $j^{\mathrm{imp}}(\mathbf{c})\sim\Gamma^{R}(\mathbf{c})\rho(\varepsilon_r,V)$. At bias voltages much lower than the height of the barrier $\varphi=(U-\varepsilon_F)$, $S_b$ can be expanded in powers of $V$:

$$S_b=q_0(b-c)\left\{1-\frac{m_0eV}{2q_0^2}\left(\frac{b-c}{w}\right)+\cdots\right\}$$

which shows that $\Gamma^{R}(\mathbf{c})\sim\exp(-S_b/\hbar)$ is an increasing function of $V$ in the vicinity of $V=0$. Hence, it leads to an increase in differential conductivity $\sigma(V)=\partial I/\partial V$ under direct bias voltage, applied to the barrier from the left to the right direction, and to a decrease in $\sigma(V)$ under reverse bias voltage. The physical meaning of such a behavior is rather obvious. From the expression for $S_b$ it follows that due to resonant levels lying close to $\varepsilon_r$ electrons tunneling under forward bias propagate through a potential barrier the effective height of which is lower than for those electrons propagating under reverse bias.

The expression for the paramagnetic impurity assisted current at finite voltages has a structure similar to Eq. (19) with Fermi distribution factors written in accordance with the general formula (17) and the integrand expression has the form given in Appendix B, where linewidths $\Gamma_{\uparrow(\downarrow)}$ have to be substituted by WKB approximation (20). In the case of magnetic impurities the above outlined mechanism of asymmetry in $I(V)$ characteristics due to the shift of resonance levels essentially contributes to the voltage dependence of TMR amplitude in question, as discussed in the next section.

## III. RESULTS AND DISCUSSION

In this section we consider the temperature and bias voltage dependencies of the conductances and TMR effect of the considered structures. We investigate the case of a Co/$Al_2O_3$/Co junction with the typical parameters that were introduced in Sec. II: $k_{\uparrow}^{F}=1.09$ Å$^{-1}$, $k_{\downarrow}^{F}=0.42$ Å$^{-1}$ are the Fermi momenta of itinerant electrons in Co, $q_0=0.56$ Å$^{-1}$ is the imaginary momentum in the barrier, $m_0=0.4$ is the effective mass in the insulator, and $w=20$ Å is its thickness. We focus on the most interesting situation when impurities are introduced in the vicinity of the left electrode at a depth $w_1$ inside the insulator layer. We chose a width $w_1=4.06$ Å which corresponds to two atomic monolayers. The essential parameter of the model which must be defined is the effective molecular field $H_z^{\mathrm{eff}}$ acting on impurity spins. One may suppose that it should exponentially decay in the depth of the barrier. We have, therefore, set it to $\mu_B H_z^{\mathrm{eff}}=5$ meV (58 K) which is two orders less than the critical temperature in bulk Co.

Consider, first, the case $T=0$. It is possible to estimate the concentration of impurity atoms so that its contribution to the resonance conductivity is comparable with the ordinary tunnel conductance of the system. One can write that the impurity density of states [see Eq. (11)] $\nu(\varepsilon_F)=N_i/A(\Delta\varepsilon)$, where $N_i$ is a total number of impurities and $\Delta\varepsilon$ is the width of its energy distribution. On the other hand, $N_i=xN$ and $N=Aw_1/a_0^3$ where $N$ is the total number of atoms in the layer which contains the impurities, $x$ is the local concentration of impurities in this volume, and $a_0$ is the lattice constant. This yields $\nu(\varepsilon_F)=x(w_1/a_0)(1/a_0^2\Delta\varepsilon)$. We introduce the characteristic concentration $x_0$ defined so that in the case of nonmagnetic impurity, the impurity conductance (11) is equal to the tunnel conductance (10) of the spin ↑ channel in the parallel magnetic configuration of the ferromagnetic layers. Such a definition leads to

$$x_0 \simeq \frac{\Delta\varepsilon}{\pi^2}\left(\frac{2m_0 a_0^2}{\hbar^2}\right)\left(\frac{w}{w-w_1}\right) \times\left(\frac{a_0}{w_1}\right)\frac{k_\uparrow^F q_0 m_0}{k_\uparrow^{F2} m_0^2+q_0^2}\,\frac{(q_0 w_1)\exp(-2q_0 w_1)}{1-\exp(-2q_0 w_1)}. \quad (22)$$

If we choose $\Delta\varepsilon = 0.2$ eV, then $x_0 = 6.5\times 10^{-5}$. The conductance of the system at $T=0$ can be extracted from the general expression (14). We suppose that for both parallel and antiparallel configurations, the left electrode has ''up'' magnetization and, hence, $H_z^{\mathrm{eff}}$ is positive in both cases. At zero temperature, all spin-flip processes are frozen and due to the above assumption, only the configuration of impurity spin with $m_s = 1$ is possible. As a result, only two resonance channels from many possible ones have nonzero contribution to conductivity, namely $|\uparrow, m_s=1\rangle \leftrightarrow |\uparrow, m_s=1\rangle$ and $|\downarrow, m_s=1\rangle \leftrightarrow |\downarrow, m_s=1\rangle$ with $m_j = 3/2$ and 1/2, respectively. From Eq. (B1) (see Appendix B), it follows that the channel with $m_j = 3/2$ gives the main contribution into the conductivity at low temperatures and ${}^P\sigma_{3/2}^{\uparrow\uparrow} \sim \Gamma_\uparrow$ and ${}^{AP}\sigma_{3/2}^{\uparrow\uparrow} \sim \Gamma_\downarrow$. So these contributions depend on the mutual orientation of the magnetization of the ferromagnetic layers, therefore they increase the total amplitude of the TMR. The total expression for $\mathrm{TMR} = (\sigma^P - \sigma^{AP})/\sigma^{AP}$ including all possible channels may be written as

$$\mathrm{TMR} = \frac{(\Gamma_\uparrow - \Gamma_\downarrow)\left[\Gamma_\uparrow - \Gamma_\downarrow + \dfrac{x}{x_0}\Gamma_\uparrow\left(1-\dfrac{1}{9}\Gamma_\downarrow/\gamma_\uparrow\right)\right]}{\Gamma_\uparrow\Gamma_\downarrow\left[2+\dfrac{x}{x_0}\left(1+\dfrac{1}{9}\Gamma_\uparrow/\gamma_\uparrow\right)\right]}, \quad (23)$$

where $x$ is concentration, $x_0$ is defined by Eq. (22), $\gamma_\uparrow = \frac{2}{3}\Gamma_\uparrow + \frac{1}{3}\Gamma_\downarrow$ and $\Gamma_{\uparrow(\downarrow)} = k_{\uparrow(\downarrow)}^F q_0^2/(k_{\uparrow(\downarrow)}^{F2} m_0^2 + q_0^2)$ are the tunneling density of states for ↑(↓) spin electrons. The dependence of TMR effect versus the polarization $P = (k_\uparrow^F - k_\downarrow^F)/(k_\uparrow^F + k_\downarrow^F)$ is shown in Fig. 3 in comparison with the nonresonant tunnel conductance at $x=0$. The total TMR amplitude is larger than the TMR due to direct tunneling, in accordance with considerations written above. For a given polarization $P = 0.44$ in case of chosen parameters, the contribution of the impurity assisted tunneling leads to a strong enhancement in TMR amplitude (typically by a factor 2, see Fig. 3).

We note, that in the case of nonmagnetic impurities distributed in the vicinity of only one contact, the resonant impurity conductance $\sigma^{\mathrm{imp}} \sim \Gamma_\uparrow + \Gamma_\downarrow$ is equal for both parallel and antiparallel configurations and, therefore, in this case, the mechanism of impurity-assisted tunneling is not able to enhance the TMR effect. The enhancement of TMR amplitude in the case of paramagnetic impurities is essentially due to the presence of a ferromagnetic exchange coupling between the magnetization in ferromagnetic electrode and the impurity spins which tends to induce a ferromagnetic order in the plane of impurities and, as a result, leads to the preference of impurity spin to be found in the quantum state with $m_s = 1$.

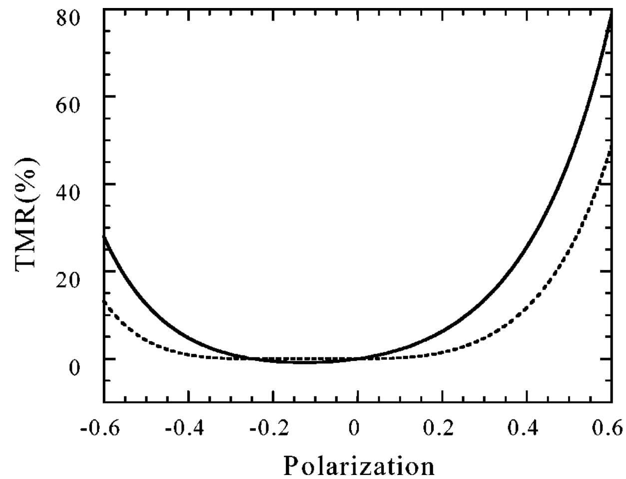


FIG. 3. Tunnel magnetoresistance at $T=0$ as a function of polarization $P = (k_\uparrow^F - k_\downarrow^F)/(k_\uparrow^F + k_\downarrow^F)$ under fixed $k_\uparrow^F = 1.09$ Å$^{-1}$. Other parameters are $q_0 = 0.56$ Å$^{-1}$, $m_0 = 0.4$. Solid line corresponds to the case of impurity concentration $x = 8\times 10^{-5}$, dashed line represents the case of absence of impurities.

The temperature dependencies of resonant conductances for parallel and antiparallel configurations in the interval from 4.2–300 K are presented in Fig. 4. In the case of parallel alignment, $\sigma_{\mathrm{imp}}^P(T)$ is nearly independent on the temperature, but in the antiparallel situation, there is a 50% increase in impurity conductance $\sigma_{\mathrm{imp}}^{AP}(T)$. This originates from the thermal excitation of both spin-flip and spin-conserving processes which are frozen at zero temperature. For AP configuration, the process $|\uparrow, m_s=0\rangle \rightarrow |\downarrow, m_s=1\rangle$ was forbidden at 0° K but now, it is allowed and gives a large contribution into the current since it is proportional to

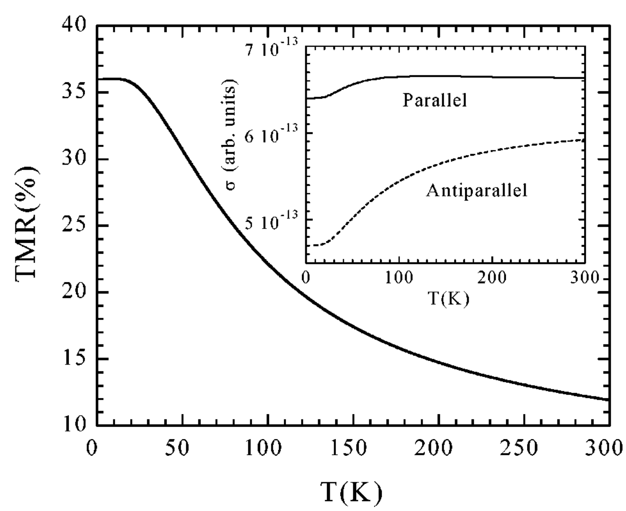


FIG. 4. Tunnel magnetoresistance as a function of the temperature. (Inset: conductance $\sigma$ for the parallel and antiparallel configurations.) The parameters are $k_\uparrow^F = 1.09$ Å$^{-1}$, $k_\downarrow^F = 0.42$ Å$^{-1}$, $q_0 = 0.56$ Å$^{-1}$, $m_0 = 0.4$. Concentration of impurities $x = 8\times 10^{-5}$.

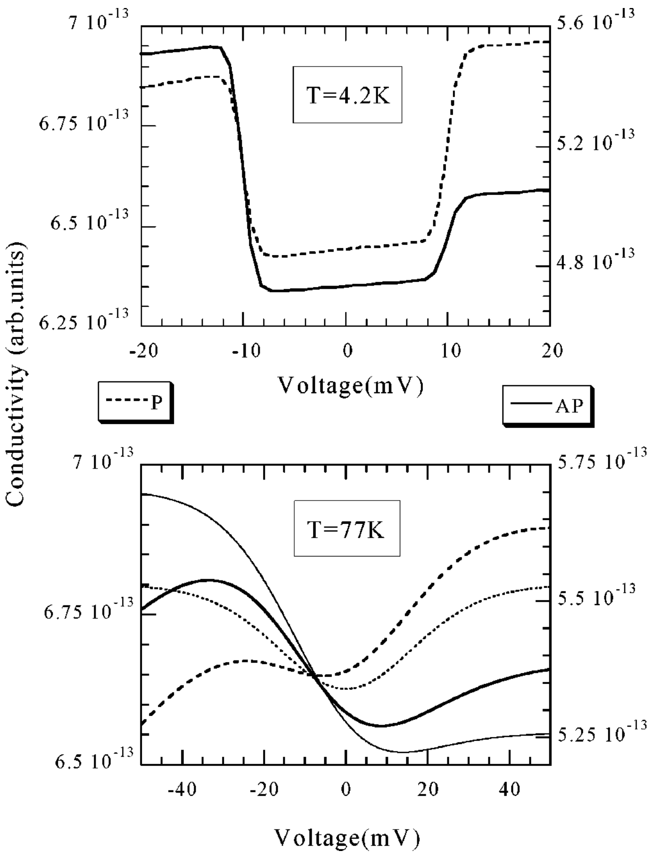


FIG. 5. Differential conductance as a function of the bias voltage at $T=4.2$ and 77 K. The parameters are $k_{\uparrow}^{F}=1.09$ Å$^{-1}$, $k_{\downarrow}^{F}=0.42$ Å$^{-1}$, $q_0=0.56$ Å$^{-1}$, $m_0=0.4$. Thick dashed and solid lines correspond to the conductance in the parallel and antiparallel configurations, respectively, calculated in the WKB approximation. For comparison, the same dependencies at $T=77$ K, calculated by approximate formulas, are indicated by thin lines. The concentration of impurities is $x=8\times10^{-5}$.

the product of the largest density of states $\Gamma_{\uparrow}\Gamma_{\uparrow}$. As a consequence, the TMR effect decreases with increasing of the temperature.

We have also calculated the dependence of the differential conductance on bias voltage according to Eqs. (18) and (19). These dependencies at $T=4.2$ K and $T=77$ K are presented in Fig. 5. A new effect is predicted: the voltage dependence of the conductance in the antiparallel alignment of magnetization in ferromagnetic layers is asymmetric under forward and reverse bias voltage when the paramagnetic impurities inside the insulator layer are distributed close to only one of the interfaces and are bound by exchange interaction with magnetization of the nearest ferromagnetic layer.

One can distinguish two different mechanisms that give rise to this asymmetrical behavior with respect to inversion of bias voltage. The first one, which we refer as zero bias anomaly, manifests itself at low voltages of the order of 10 mV (for particular chosen parameters in our model) and is strongly pronounced only at low temperatures (see Fig. 5, the case of $T=4.2$ K). It originates from the excitations of spin-flip processes at the impurity sites. One may look at the general expression (18) and consider the case of low temperature. An electron undergoing spin-flip scattering, may transfer an amount of energy $\omega_0=2\mu_B H_z^{\mathrm{eff}}$ to the impurity spin thus exiting it at an higher energy level or on the contrary may acquire this quantum of energy from it. The latter process is impossible at low temperature. The former one is possible only if an electron moving, say, from the left contact possesses an excess energy of at least $\omega_0$ with respect to Fermi level in the right contact. The only one process that contributes to this anomaly at low temperature is $\phi_{1/2}^{\downarrow}\to\phi_{1/2}^{\uparrow}$ [see Eq. (15)]. For antiparallel alignment of the magnetization, its quantum-mechanical probability is proportional to ${}^{AP}\sigma_{1/2}^{\downarrow\uparrow}\sim\frac{2}{9}\Gamma_{\downarrow}^{2}/\gamma_{\uparrow}$ for electrons moving from the left ferromagnetic layer into the right one and is proportional to ${}^{AP}\sigma_{1/2}^{\uparrow\downarrow}\sim\frac{2}{9}\Gamma_{\uparrow}^{2}/\gamma_{\uparrow}$ in the case of electrons moving from the right to the left. For parallel configuration of magnetizations, these probabilities are equal in both directions and are proportional to ${}^{P}\sigma_{1/2}^{\downarrow\uparrow}={}^{P}\sigma_{1/2}^{\uparrow\downarrow}\sim\frac{2}{9}\Gamma_{\downarrow}\Gamma_{\uparrow}/\gamma_{\uparrow}$. As a result, the zero bias anomaly at $T=4.2$ K looks asymmetric in the case of antiparallel configuration and is symmetric in the case of parallel alignment of magnetizations.

The differential conductances as a functions of the bias voltage at $T=77$ K have been calculated using two different approximations. Thick dashed and solid lines correspond to the conductances in the parallel and antiparallel configurations, respectively, that have been calculated by means of WKB approximation in accordance with expressions (17) and (19). For the sake of comparison, the same dependencies, indicated by thin lines, have been calculated by using the approximate formulas (18), where the dependence of $\hat{t}$-matrix elements on the applied voltage has been neglected. The latter curves demonstrate the only zero bias anomaly discussed above, which is substantially smoothed, compared with the case of $T=4.2$ K. On the contrary, the WKB scheme of calculation takes into account the variation of the potential profile inside the insulating barrier under applied bias voltage. In view of this, the differential conductances calculated by this scheme exhibit a tendency to increase at the direct bias voltage and to decrease at the reverse one. As was shown above (see Sec. II D), this behavior originates from the shift of the resonant levels inside the insulator due to externally applied electric field. This second mechanism in the origin of nonlinear voltage dependence of impurity-assisted conductance does not relate with the excitation of spin-flip processes. It becomes apparent at voltages of the order of 50 mV and leads to asymmetric voltage bias dependencies in both cases of parallel and antiparallel configurations.

Finally, the TMR amplitude as a function of bias voltage is shown in Fig. 6 for a broad range of applied voltage. Its nonlinear and asymmetric behavior in the range of 0.2 V originates from the asymmetry of the shifts of resonant impurity levels with respect to forward and inverse bias. The low bias voltage anomaly at 10 mV is also strongly pronounced at the curve corresponding to 4.2 K. The relative contribution of the impurity-assisted conductance to the total current of electrons decreases when the value of applied bias voltage exceeds the half width of impurity band $\Delta\varepsilon/2$

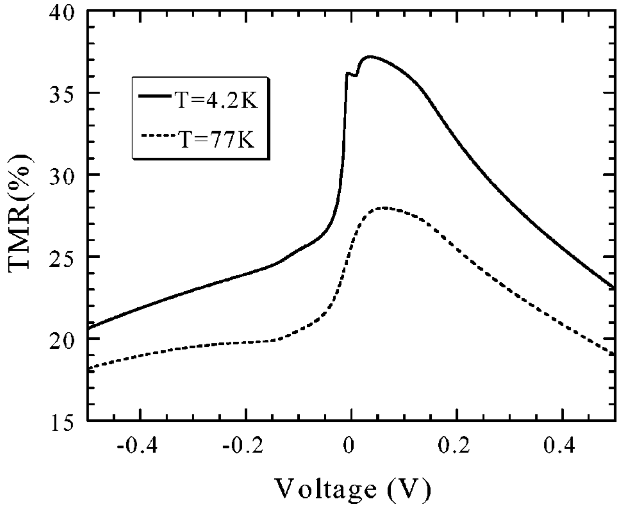


FIG. 6. Tunnel magnetoresistance as a function of the bias voltage. Solid line: $T=4.2$ K, dashed line: $T=77$ K. The parameters are $k_{\uparrow}^{F}=1.09$ Å$^{-1}$, $k_{\downarrow}^{F}=0.42$ Å$^{-1}$, $q_0=0.56$ Å$^{-1}$, $m_0=0.4$. The concentration of impurities is $x=8\times10^{-5}$.

$=0.1$ eV. Therefore, the TMR amplitude drops to value $\simeq 20\%$ at 0.5 V corresponding primarily to the pure tunnel conductance.

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## APPENDIX A

In this appendix we briefly demonstrate the details of the derivation Eq. (4) for the impurity conductance in the second order of the perturbation theory. In the Kubo formalism of a linear response the real part of a frequency-dependent conductivity is given by the expression[16]

$$\mathrm{Re}\,\sigma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega)=\frac{1-e^{-\beta\omega}}{2\omega}\Gamma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega).$$

Here $\beta=1/k_BT$; $\mu$, $\rho$ denote electron spins and $\Gamma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega)$ is a Fourier transform of the current-current correlation function

$$\Gamma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega)=\int_{-\infty}^{+\infty}\langle j_\rho(\mathbf{r}',t')j_\mu(\mathbf{r},t)\rangle e^{i\omega(t-t')}d(t-t'),$$

where $\langle\cdots\rangle$ denote the quantum statistical averaging. For our purposes we have calculated the static conductivity $\sigma_{\mu\rho}(\mathbf{r},\mathbf{r}')=(\beta/2)\Gamma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega)|_{\omega=0}$ by means of the Keldysh method of nonequilibrium Green functions.[17] In this approach a four-component matrix Green function

$$G_\mu(\varepsilon)=\begin{pmatrix}G_\mu^{--}(\varepsilon) & G_\mu^{-+}(\varepsilon)\\ G_\mu^{+-}(\varepsilon) & G_\mu^{++}(\varepsilon)\end{pmatrix}=\begin{pmatrix}G_\mu^{T}(\varepsilon) & G_\mu^{<}(\varepsilon)\\ G_\mu^{>}(\varepsilon) & G_\mu^{\tilde{T}}(\varepsilon)\end{pmatrix}\tag{A1}$$

is introduced into consideration (two equivalent forms of notation are presented). It is remarkable that initial equilibrium Green functions of the unperturbed system for the given chemical potential $\varepsilon_F$ can be expressed in terms of only retarded and advanced propagators $G^R(\varepsilon)$ and $G^A(\varepsilon)$

$$\begin{aligned}G_\mu^T(\varepsilon)&=f(\varepsilon-\varepsilon_F)G_\mu^A(\varepsilon)+[1-f(\varepsilon-\varepsilon_F)]G_\mu^R(\varepsilon),\\ G_\mu^{\tilde{T}}(\varepsilon)&=-[1-f(\varepsilon-\varepsilon_F)]G_\mu^A(\varepsilon)-f(\varepsilon-\varepsilon_F)G_\mu^R(\varepsilon),\\ G_\mu^{<}(\varepsilon)&=f(\varepsilon-\varepsilon_F)[G_\mu^A(\varepsilon)-G_\mu^R(\varepsilon)],\\ G_\mu^{>}(\varepsilon)&=-[1-f(\varepsilon-\varepsilon_F)][G_\mu^A(\varepsilon)-G_\mu^R(\varepsilon)],\end{aligned}\tag{A2}$$

where $f(\varepsilon-\varepsilon_F)$ is the Fermi distribution function. In the same way the set of possible spin-spin correlation functions in the energy representation of the type $\langle\langle S_+|S_-\rangle\rangle_\omega$ and $\langle\langle S_z|S_z\rangle\rangle_\omega$ we denote as matrices $D_{xy}(\omega)$ and $D_{zz}(\omega)$ which have the same structure as the matrix (A1). In the case of noninteracting system corresponding to the ''isolated'' impurity spin in the ''external'' magnetic field $H_z^{\mathrm{eff}}$ the explicit form of, e.g., $D_{xy}(\omega)$ is written as

$$\begin{aligned}D_{xy}^T(\omega)&=\frac{\langle S_+S_-\rangle}{\omega-2\mu_BH_z^{\mathrm{eff}}+i0}-\frac{\langle S_-S_+\rangle}{\omega-2\mu_BH_z^{\mathrm{eff}}-i0},\\ D_{xy}^{\tilde{T}}(\omega)&=\frac{\langle S_-S_+\rangle}{\omega-2\mu_BH_z^{\mathrm{eff}}+i0}-\frac{\langle S_+S_-\rangle}{\omega-2\mu_BH_z^{\mathrm{eff}}-i0},\\ D_{xy}^{>}(\omega)&=-2\pi i\,\delta(\omega-2\mu_BH_z^{\mathrm{eff}})\langle S_+S_-\rangle,\\ D_{xy}^{<}(\omega)&=-2\pi i\,\delta(\omega-2\mu_BH_z^{\mathrm{eff}})\langle S_-S_+\rangle.\end{aligned}\tag{A3}$$

The construction of diagrams in the framework of the Keldysh approach include the additional symbols $+$ and $-$ in all vertex points of the graph so that each line is associated with the corresponding component of the electron or spin Green function. In this sense the current-current correlation function $\Gamma_{\mu\rho}(\mathbf{r},\mathbf{r}',\omega)$ is related with the series of diagrams starting from the symbol $+$ at the point $\mathbf{r}'$ and ending by the symbol $-$ at the point $\mathbf{r}$. This fact is schematically presented in Eq. (2) in the form of a product of two corresponding electron Green functions. Actually, substituting them by zero-order Green functions (A2) one will obtain the ''bubble'' part of the current-current correlator corresponding to the nonresonant part of the conductance $\sigma_0(T)$ [Eq. (3)]. The rest of the series, known as the ''vertex'' correction, determines the impurity-assisted conductance $\sigma_{\mathrm{imp}}(T)$. In the second order of perturbation theory there exist four different diagrams contributing to it. Two of them are shown in Fig. 2 and other ones can be obtained from the former by substituting spin up ($\uparrow$) by spin down ($\downarrow$) and vice versa. The explicit analytical expression, for example, for the diagram in Fig. 2(b), is written as follows

$$\Gamma^{(2)}_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}',0)=\sum_{\alpha,\beta=\pm}(-\alpha\beta)\frac{J^2e^2}{\hbar}\int\int_{-\infty}^{+\infty}\frac{d\varepsilon d\omega}{(2\pi)^2}\,iD^{\alpha\beta}_{xy}(\omega)\times G^{+\alpha}_{\downarrow}\left(\mathbf{c},\mathbf{r}',\varepsilon+\frac{\omega}{2}\right)\frac{\overleftrightarrow{\nabla}_{\mathbf{r}'}}{2m}G^{\beta+}_{\downarrow}\left(\mathbf{r}',\mathbf{c},\varepsilon+\frac{\omega}{2}\right)\times G^{\alpha-}_{\uparrow}\left(\mathbf{c},\mathbf{r},\varepsilon-\frac{\omega}{2}\right)\frac{\overleftrightarrow{\nabla}_{\mathbf{r}}}{2m}G^{-\beta}_{\uparrow}\left(\mathbf{r},\mathbf{c},\varepsilon-\frac{\omega}{2}\right),$$

where the sum over $\alpha$ and $\beta$ takes into account four possible Keldysh diagrams corresponding to this graph. But one can easy see that two terms, containing $D^{--}_{xy}(\omega)$ and $D^{++}_{xy}(\omega)$, are not essential since they cancel due to the asymmetric gradient operation $\overleftrightarrow{\nabla}_{\mathbf{r}}$ and $\overleftrightarrow{\nabla}_{\mathbf{r}'}$, respectively. The other two terms after substituting Eqs. (A2) and (A3) and integrating over $\omega$ may be rewritten as

$$\Gamma^{(2)}_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}',0)=\frac{2J^2e^2}{\pi\hbar}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{2\pi}\Phi^L_{\uparrow}(\mathbf{c},\varepsilon)\Phi^R_{\downarrow}(\mathbf{c},\varepsilon)\{f_{\uparrow}(\varepsilon-\mu_BH^{\mathrm{eff}}_z)[1-f_{\downarrow}(\varepsilon+\mu_BH^{\mathrm{eff}}_z)]\langle S_-S_+\rangle+f_{\downarrow}(\varepsilon+\mu_BH^{\mathrm{eff}}_z)[1-f_{\uparrow}(\varepsilon-\mu_BH^{\mathrm{eff}}_z)]\langle S_+S_-\rangle\}. \tag{A4}$$

Here we suppose that $r<c<r'$ and introduce the hopping probabilities of an electron from the bulk itinerant state to the impurity level

$$\Phi^L_{\uparrow}(\mathbf{c},\varepsilon)=G^A_{\uparrow}(\mathbf{c},\mathbf{r},\varepsilon)\frac{\overleftrightarrow{\nabla}_{\mathbf{r}}}{4mi}G^R_{\uparrow}(\mathbf{r},\mathbf{c},\varepsilon)|_{\mathbf{r}=a},$$

$$\Phi^R_{\downarrow}(\mathbf{c},\varepsilon)=-G^R_{\downarrow}(\mathbf{r}',\mathbf{c},\varepsilon)\frac{\overleftrightarrow{\nabla}_{\mathbf{r}'}}{4mi}G^A_{\downarrow}(\mathbf{c},\mathbf{r}',\varepsilon)|_{\mathbf{r}'=b}.$$

Straightforward calculations show that these quantities do not explicitly depend on $\mathbf{r}$ and $\mathbf{r}'$ and hence $\Gamma^{(2)}_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}',0)$ is determined only by the position ofthe impurity $\mathbf{c}$. We also note that two terms in Eq. (A4), corresponding to the direct and inverse process, respectively, in fact are equal to each other after performing the thermodynamic averaging that expresses the principle of the detailed equilibrium in the system. The structure of the expression (A4) is similar to that of Eq. (4). Equation (A4) will reproduce this final result if one substitutes the scattering amplitudes $\langle S_+S_-\rangle$ and $\langle S_-S_+\rangle$ calculated in the second order of $J$ by the average product of corresponding $t$ matrices $\langle\hat{t}_+(\varepsilon)\hat{t}_-(\varepsilon)\rangle$ and $\langle\hat{t}_-(\varepsilon)\hat{t}_+(\varepsilon)\rangle$. The validity of this approximation is discussed in the main text and it is justified in case of neglecting of a double occupancy of electrons with different spins at the same impurity center.

## APPENDIX B

Let $w_1=c-a$ and $w_2=b-c$ be the position of impurity with respect to the left and right interfaces, respectively, and $w=b-a$ be the width of the insulator layer. We introduce tunneling densities of states for spin $\uparrow(\downarrow)$ electrons $\Gamma_{\uparrow(\downarrow)}=k^F_{\uparrow(\downarrow)}q_0^2/(k^F_{\uparrow(\downarrow)}m_0^2+q_0^2)$ and denote $\gamma_\uparrow=\frac{2}{3}\Gamma_\uparrow+\frac{1}{3}\Gamma_\downarrow$, $\gamma_\downarrow=\frac{1}{3}\Gamma_\uparrow+\frac{2}{3}\Gamma_\downarrow$. Then, the position-dependent quantum-mechanical probabilities $\sigma^{\mu\rho}_{m_j}(c)$ can be found as follows.

(a) In the case of parallel configuration

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{3/2(-3/2)}(c)=\frac{\Gamma^2_{\uparrow(\downarrow)}e^{-2q_0w}/(w_1w_2)}{\Gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_1}}{w_1}+\Gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{1/2(-1/2)}(c)=\frac{4}{9}\frac{\Gamma^2_{\uparrow(\downarrow)}e^{-2q_0w}/(w_1w_2)}{\gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_1}}{w_1}+\gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{-1/2(1/2)}(c)=\frac{1}{9}\frac{\Gamma^2_{\uparrow(\downarrow)}e^{-2q_0w}/(w_1w_2)}{\gamma_{\downarrow(\uparrow)}\frac{e^{-2q_0w_1}}{w_1}+\gamma_{\downarrow(\uparrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\downarrow\uparrow}_{1/2}(c)=\sigma^{\uparrow\downarrow}_{1/2}(c)=\frac{2}{9}\frac{\Gamma_\uparrow\Gamma_\downarrow e^{-2q_0w}/(w_1w_2)}{\gamma_\uparrow\frac{e^{-2q_0w_1}}{w_1}+\gamma_\uparrow\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\downarrow}_{-1/2}(c)=\sigma^{\downarrow\uparrow}_{-1/2}(c)=\frac{2}{9}\frac{\Gamma_\uparrow\Gamma_\downarrow e^{-2q_0w}/(w_1w_2)}{\gamma_\downarrow\frac{e^{-2q_0w_1}}{w_1}+\gamma_\downarrow\frac{e^{-2q_0w_2}}{w_2}}. \tag{B1}$$

(b) In the case of antiparallel configuration

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{3/2(-3/2)}(c)=\frac{\Gamma_\uparrow\Gamma_\downarrow e^{-2q_0w}/(w_1w_2)}{\Gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_1}}{w_1}+\Gamma_{\downarrow(\uparrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{1/2(-1/2)}(z)=\frac{4}{9}\frac{\Gamma_\uparrow\Gamma_\downarrow e^{-2q_0w}/(w_1w_2)}{\gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_1}}{w_1}+\gamma_{\downarrow(\uparrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\uparrow(\downarrow\downarrow)}_{-1/2(1/2)}(z)=\frac{1}{9}\frac{\Gamma_\uparrow\Gamma_\downarrow e^{-2q_0w}/(w_1w_2)}{\gamma_{\downarrow(\uparrow)}\frac{e^{-2q_0w_1}}{w_1}+\gamma_{\uparrow(\downarrow)}\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma^{\uparrow\downarrow(\downarrow\uparrow)}_{1/2}(z)=\frac{2}{9}\frac{\Gamma^2_{\uparrow(\downarrow)}e^{-2q_0w}/(w_1w_2)}{\gamma_\uparrow\frac{e^{-2q_0w_1}}{w_1}+\gamma_\downarrow\frac{e^{-2q_0w_2}}{w_2}},$$

$$\sigma_{-1/2}^{\uparrow\downarrow(\downarrow\uparrow)}(z)=\frac{2}{9}\frac{\Gamma^2_{\uparrow(\downarrow)}e^{-2q_0w}/(w_1w_2)}{\gamma_\downarrow\dfrac{e^{-2q_0w_1}}{w_1}+\gamma_\uparrow\dfrac{e^{-2q_0w_2}}{w_2}}. \qquad \text{(B2)}$$

The statistical probabilities $P_{m_j}^{\mu\rho}(h)$ are independent of the configuration of the system. We denote $h=\mu_B H_z^{\text{eff}}/kT$ and $Z=2\cosh(2h)+1$, then

$$P_{3/2}^{\uparrow\uparrow}(h)=P_{1/2}^{\downarrow\downarrow}(h)=Z^{-1}e^{2h},\quad P_{1/2}^{\uparrow\uparrow}(h)=P_{-1/2}^{\downarrow\downarrow}(h)=Z^{-1},$$

$$P_{-1/2}^{\uparrow\uparrow}(h)=P_{-3/2}^{\downarrow\downarrow}(h)=Z^{-1}e^{-2h},$$

$$P_{1/2}^{\uparrow\downarrow}(h)=P_{1/2}^{\downarrow\uparrow}(h)=Z^{-1}\frac{he^{h}}{\sinh(h)},$$

$$P_{-1/2}^{\uparrow\downarrow}(h)=P_{-1/2}^{\downarrow\uparrow}(h)=Z^{-1}\frac{he^{-h}}{\sinh(h)}. \qquad \text{(B3)}$$

## APPENDIX C

The nontrivial functions $I_{m_j}^{\mu\rho}$ are written as

$$I_{1/2}^{\downarrow\uparrow}(V,H_z^{\text{eff}})=\frac{(eV-2\mu_B H_z^{\text{eff}})(e^{eV/kT}-1)}{(e^{(eV-2\mu_B H_z^{\text{eff}})/kT}-1)Z},$$

$$I_{1/2}^{\uparrow\downarrow}(V,H_z^{\text{eff}})=\frac{(eV+2\mu_B H_z^{\text{eff}})(e^{eV/kT}-1)e^{2\mu_B H/kT}}{(e^{(eV+2\mu_B H_z^{\text{eff}})/kT}-1)Z},$$

$$I_{-1/2}^{\uparrow\downarrow}(V,H_z^{\text{eff}})=\frac{(eV+2\mu_B H_z^{\text{eff}})(e^{eV/kT}-1)}{(e^{(eV+2\mu_B H_z^{\text{eff}})/kT}-1)Z},$$

$$I_{-1/2}^{\downarrow\uparrow}(V,H_z^{\text{eff}})=\frac{(eV-2\mu_B H_z^{\text{eff}})(e^{eV/kT}-1)e^{-2\mu_B H/kT}}{(e^{(eV-2\mu_B H_z^{\text{eff}})/kT}-1)Z}.$$

All the other ones, not written above, are equal to $eV\times P_{m_j}^{\mu,\mu}(h)$.


[1] J.S. Moodera, L.R. Kinder, T.M. Wong, and R. Meservey, Phys. Rev. Lett. **74**, 3273 (1995).

[2] T. Miyazaki and N. Tezuka, J. Magn. Magn. Mater. **139**, L231 (1995).

[3] W.J. Gallagher *et al.*, J. Appl. Phys. **81**, 3741 (1997).

[4] J.C. Słonczewski, Phys. Rev. B **39**, 6995 (1989).

[5] A. Vedyayev, N. Ryzhanova, C. Lacroix, L. Giacomoni, and B. Dieny, Europhys. Lett. **39**, 219 (1997).

[6] A. Vedyayev, N. Ryzhanova, R. Vlutters, and B. Dieny, Europhys. Lett. **46**, 808 (1999).

[7] I.M. Lifshitz and V. Ya. Kirpichenkov, Zh. Éksp. Teor. Fiz. **77**, 989 (1979) [Sov. Phys. JETP **50**, 499 (1979)].

[8] A.I. Larkin and K.A. Matveev, Zh. Éksp. Teor. Fiz. **93**, 1030 (1987) [Sov. Phys. JETP **66**, 580 (1987)].

[9] A.M. Bratkovsky, Pis'ma Zh. Éksp. Teor. Fiz. **65**, 430 (1997) [JETP Lett. **65**, 452 (1997)].

[10] E. Yu. Tsymbal and D.G. Pettifor, Phys. Rev. B **58**, 432 (1998).

[11] H. Itoh, T. Kumazaki, J. Inoe, and S. Maekawa, Jpn. J. Appl. Phys. **37**, 554 (1998).

[12] F. Guinea, Phys. Rev. B **58**, 9212 (1998).

[13] R. Jansen and J.C. Lodder, Phys. Rev. B **61**, 5860 (2000). In this work the spin-dependent polarized densities of resonant states $\nu_\uparrow$ and $\nu_\downarrow$ have been introduced into the consideration. However, no physical mechanism underlying these phenomenological quantities has been proposed by the authors. We may note that the term ''spin-polarized resonant tunneling'' was proposed in Ref. 14. In the latter work the tunneling through the double-barrier tunnel structure has been investigated. The case of a triple-barrier junction was later investigated in Ref. 19. In these structures the spin-polarized resonant density of states exists in fact, but it arises due to the formation of so-called quantum-well states.

[14] Xiangdong Zhang, Bo-Zhang Li, Gang Sun, and Fu-Cho Pu, Phys. Rev. B **56**, 5484 (1997).

[15] S. Zhang, P. Levy, A.C. Marley, and S.S.P. Parkin, Phys. Rev. Lett. **79**, 3744 (1997).

[16] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II. Nonequilibrium Statistical Mechanics* (Springer, Berlin, 1985).

[17] E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics, Course of Theoretical Physics*, Vol. 10 (Pergamon, Oxford, 1981).

[18] L. D. Landau and I. M. Lifshitz, *Quantum Mechanics, Course of Theoretical Physics*, Vol. 3 (Pergamon, Oxford, 1977).

[19] A. Vedyayev, N. Ryzhanova, R. Vlutters, B. Dieny, and N. Strelkov, J. Phys.: Condens. Matter **12**, 1797 (2000).