PHYSICAL REVIEW B **77**, 024410 (2008)

Theory of interlayer magnetic coupling in nanostructures with disordered interfaces

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(Received 2 October 2007; revised manuscript received 22 November 2007; published 10 January 2008)

Multiple scattering theory of interlayer coupling in nanostructures with disordered alloylike interfaces is developed. Interface-localized potential responsible for the specular electron reflection from a perfect interface (potential step) is found in the framework of multiple scattering theory based on Green's functions approach. This allowed obtaining of a general expression relating the interlayer coupling energy to electronic density of states change due to interferences of electronic waves resulting from multiple reflections at disordered interfaces. In the case of a small spacer electron confinement (small scattering), the interlayer exchange coupling between two ferromagnets separated by a nonmagnetic spacer is found in the coherent potential approximation for electrons scattering at the disordered interfaces. The influence of disorder on the oscillating with a metallic spacer thickness exchange coupling is analyzed. The main effect is found to be a phase shift and amplitude change of these oscillations with the change of the parameters describing specular and diffuse spin-dependent electron scattering caused by the interfacial disorder.

DOI: 10.1103/PhysRevB.77.024410 PACS number(s): 73.21.Ac, 72.25.Mk, 73.40.Gk, 85.75.−d

I. INTRODUCTION

Artificial structures consisting of alternating magnetic and nonmagnetic layers, each of a few atomic layers thick, have been attracting a good deal of interest especially since the discovery of the giant magnetoresistance (GMR)[1] and tunneling magnetoresistance (TMR)[2,3] effects. These structures exhibit GMR and TMR under certain conditions. One of them is a possibility to switch between antiparallel and parallel alignments of magnetization vectors of ferromagnetic layers in a multilayer or a sandwich. The antiferromagnetic coupling of Fe films separated by a Cr spacer was first observed in Ref. 4. Later, a spectacular periodic dependence of the sign of the interlayer exchange interaction between ferromagnetic layers on the metallic nonmagnetic layer thickness was discovered in Refs. 5 and 6. The latter effect as well as the effect of interlayer exchange coupling across nonmetallic layers, first studied in Ref. 7 for Fe films separated by amorphous Si, have been a subject of intensive research in the last years. In contrast to the case of a metal spacer, the coupling through a nonmetal spacer is nonoscillatory, decays with the spacer thickness, and increases with temperature increase.

A great number of studies have been performed on the interlayer coupling via a metal spacer with special attention to its oscillatory behavior. We cite here the most comprehensive, from our point of view, theoretical investigations by Bruno[8] and Stiles,[9] where all other suitable references can be found. In these papers, a general approach to the problem of interlayer coupling in terms of the quantum interference due to the (spin-dependent) specular reflections of electron Bloch waves at the perfect paramagnet-ferromagnet interfaces has been proposed. This interference of the electron waves results in a change of the density of states in the spacer and leads to the oscillatory behavior of interlayer coupling energy with the spacer thickness (for metal spacer). In addition to being very physically transparent, this approach embodies all the previously suggested models [e.g., Rudermar-Kittel-Kasuya-Yosida (RKKY) model[10]] and allows treating on the equal footing of both the metal and insulator spacer cases[8] (coupling through a tunneling barrier was first considered by Slonczewski[11]).

It should be stressed, however, that the basic approach by Bruno and Stiles treats the interfaces in nanostructures as the perfect ones. In this case the electron reflections at and transmissions through the interfaces are $\mathbf{k}_\parallel$ conserved due to the translational invariance of the interface ($\mathbf{k}_\parallel$ is an electron wave vector parallel to the interfaces). However, the real interfaces are disordered. They are characterized by roughness (long-range imperfections, compared to the electron mean free path l, which do not break the in-plane translational invariance) and intermixing (short-range imperfections breaking the in-plane translational invariance). The interface roughness can be associated with long-range deviation of either the thickness or the crystallographic orientations of the layers, whereas the intermixing of different layers in the interface region can be modeled by an alloy of short-range scatterers. There have been a number of theoretical and experimental studies of interface roughness and its influence on the GMR and other phenomena. For instance, the influence of interface roughness on GMR was studied in Refs. 12 and 13, where the authors introduced a model treating interfaces as nonflat ones; *ab initio* calculations for the interlayer exchange coupling in the presence of an interfacial roughness and interdiffusion were performed in Ref. 14. However, to the best of our knowledge, no general theoretical treatment of the problem of interlayer coupling in the case of disordered interfaces has been published to date.

The essential problem is then how to generalize the basic approach of Refs. 8 and 9 to the case of disordered interfaces, and whether and how the predictions of these theories for the perfect interfaces are affected by interfacial disorder. Advances in both molecular dynamics simulations and experimental techniques have provided crucial information on the structure of multilayer interface regions.[15,16] These studies show that the interfaces in a number of technologically important multilayers can be viewed as locally crystalline with interdiffusion of different atomic species within a few layers of the interface. In a recently published paper,[17] the authors stress that for a proper description of the interface structure and interpretation of the experimental data on the GMR effect and interlayer coupling, the atomic scale disorder, which is typically caused by an alloying process (intermixing of different materials at the interface), should be taken into consideration. They suggest a microscopic mechanism of the interface alloying, and provide a description of interface roughness and its correlation with the GMR effect and interlayer coupling in Fe/Cr multilayers.

In the present paper, we develop a general approach to the problem of interlayer coupling in real nanostructures with disordered interfaces. Based on the above-mentioned results, we adopt for the interface structure a model of disordered alloy made of atoms of the adjacent layers. When an interfacial disorder is present, the in-plane component of electron wave vector may no longer be conserved and the influence of disorder on the specular and arising diffuse scattering of electrons at the interface needs to be studied. Transmission and reflection amplitudes for an electron striking a disordered interface at an arbitrary angle have been found in a closed analytical form in Ref. 18 in the self-consistent single-site coherent potential approximation (CPA) for interfacial disorder and the effective-mass approximation (EMA) for the electron spectra in different layers. The EMA is suitable for *s* and majority *d* electrons in some important ferromagnetic materials (Co, Ni) and now actively studied diluted magnetic semiconductors (DMS), which are viewed as promising materials for spintronics.

In Sec. II of this paper, the general, based on the Green functions formalism, scattering theory approach to the reflection of spacer electrons from two interfaces is outlined. Necessary for this approach, localized (at an interface) potential, responsible for reflection from a perfect interface (potential step), is obtained in Sec. II A. This further allows introducing a combined potential describing the scattering due to both interface potential profile change and disorder caused by the atoms of adjacent layers mixing at the interface. As a result, a general expression for the electron energy change (the coupling energy) caused by the interferences of electronic waves due to multiple reflections of the spacer electrons from the disordered interfaces is obtained in Sec. II B. In Sec. III, this result is used to get the exchange coupling energy (in the case of small reflection amplitudes) for a trilayer made of two ferromagnets divided by a nonmagnetic spacer. The coherent potential approximation (CPA) is used for electron scattering at a disordered interface. Parameters describing the influence of disorder on the exchange coupling are introduced, and the change of the oscillating with the spacer thickness exchange coupling (in the case of a metallic spacer) as a function of these parameters is analyzed and plotted. The results are summarized in Sec. IV.

II. SCATTERING THEORY APPROACH TO REFLECTION FROM INTERFACES

The general approach developed in Refs. 9 and 8 suggests, quite naturally, to relate the interlayer coupling to the electrons' energy (thermodynamic potential) change due to quantum interferences of electronic waves in a spacer layer. Consider a multilayer made of (generally different) magnetic layers separated by nonmagnetic layers. The thicknesses of magnetic layers are supposed (for simplicity) to be larger than the electronic mean free path l, whereas the spacer (nonmagnetic layer) thickness is less than l. In this case we may consider the interlayer coupling between magnetic layers through the spacer taking into account interferences of electronic waves (as a reason for coupling) in the spacer only. Thus it is sufficient to consider a system of two magnetic layers parallel to the (x,y) plane with interfaces at $z=0$ and $z=d$ and separated by a nonmagnetic spacer (with thickness d). Electrons traveling in the spacer experience repeated reflections from the nonmagnetic-magnetic interfaces which may lead to quantum interferences of electronic waves and to a corresponding change of the electron density of states and energy. The latter leads to the interlayer coupling.

The appropriate (for considering the electrons' interferences) Hamiltonian of this system may be written as

$$H=H_0+V^0+V^d, \tag{1}$$

where H_0 is the spacer electrons' Hamiltonian and V^0 and V^d represent the scattering potentials of the interfaces located at $z=0$ and $z=d$, respectively. These potentials stem from the conduction-band steplike profile $U(z)$ of the trilayer (forming a potential well or barrier for spacer electrons) and interfacial disorder which will be modeled by the short-range scattering centers located in the interface plane (x,y). For the perfect interfaces, the scattering potential caused by $U(z)$ depends only on the coordinate normal to the layers, and the in-plane component $\mathbf{k}_\parallel$ of the electron wave vector is a good quantum number. Thus from the symmetry consideration, the electron reflection amplitudes for an electron state of wave vector $\mathbf{k}=(k_\perp,\mathbf{k}_\parallel)$ depends only on the perpendicular to the interfaces component $k_\perp$, which, of course, depends on the electron energy and $\mathbf{k}_\parallel$. Therefore for each $\mathbf{k}_\parallel$ (angle of electron incidence on the interface) we have a one-dimensional problem of the electron multiple scatterings from the interfaces (the scattering amplitudes are diagonal in the $\mathbf{k}_\parallel$ representation). For disordered interfaces, when $\mathbf{k}_\parallel$ may no longer be conserved, the electron reflection (and transmission) amplitude is not diagonal in the $\mathbf{k}_\parallel$ representation, but the needed average (over all configurations of the mixed at an interface atoms) electronic density of states remains diagonal in the $\mathbf{k}_\parallel$ representation. It follows (see below) that one may consider a one-dimensional problem of the quantum interferences in the spacer for an electron with given $\mathbf{k}_\parallel$ (leading to the electron density of states change) and then sum up the result over in-plane electron wave vectors to get a three-dimensional problem solution.

The thermodynamic grand potential change $\Delta\Phi$ associated with the electronic density of states change $\Delta n(\varepsilon)$ at temperature T is

$$\Delta\Phi=-k_BT\int_{-\infty}^{\infty}\Delta n(\varepsilon)\ln\left[1+\exp\left(\frac{\varepsilon_F-\varepsilon}{k_BT}\right)\right]d\varepsilon, \tag{2}$$

where ε_F is the Fermi energy.

The density of states $n(\varepsilon)$ is conveniently expressed in terms of the Green function $G(\varepsilon)$ corresponding to the system Hamiltonian (1) as

$$n(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\mathrm{Tr}\langle G(\varepsilon + i0^+)\rangle,$$

$$G(\varepsilon) = (\varepsilon - H_0 - V^0 - V^d)^{-1}, \tag{3}$$

where $\langle\cdots\rangle$ denotes a configurational average over all the interface scatterers (impurities) configurations and $i0^+$ is infinitesimal imaginary energy. Note that the averaged Green function is diagonal with respect to $\mathbf{k}_\parallel$ [we do not show in Eq. (3) explicitly the corresponding matrix element of $\langle G(\varepsilon + i0^+)\rangle$ in $\mathbf{k}_\parallel$ representation for brevity] because the averaging restores the translational invariance of a disordered interface. Treating $V^0 + V^d$ as perturbation, the Green function $G(\varepsilon)$ may be expressed as

$$G(\varepsilon) = G_0(\varepsilon) + \Delta G^0(\varepsilon) + \Delta G^d(\varepsilon) + \Delta G^{0d}(\varepsilon). \tag{4}$$

Here,

$$G_0(\varepsilon) = (\varepsilon - H_0)^{-1},$$

$$\Delta G^{0(d)}(\varepsilon) = G_0(\varepsilon)T^{0(d)}(\varepsilon)G_0(\varepsilon),$$

$$\Delta G^{0d}(\varepsilon) = G_0T^0(1 - G_0T^dG_0T^0)^{-1}G_0T^d(1 + G_0T^0)G_0 + G_0T^d(1 - G_0T^0G_0T^d)^{-1}G_0T^0(1 + G_0T^d)G_0,$$

$$T^{0(d)}(\varepsilon) = V^{0(d)} + V^{0(d)}G_0(\varepsilon)V^{0(d)} + V^{0(d)}G_0(\varepsilon)V^{0(d)}G(\varepsilon)V^{0(d)} + \cdots = V^{0(d)}[1 - G_0(\varepsilon)V^{0(d)}]^{-1}, \tag{5}$$

where $G_0(\varepsilon)$ represents the electron propagation in the spacer material, the t-matrix $T^{0(d)}(\varepsilon)$ describes multiple reflections from the interface potential $V^{0(d)}$, $\Delta G^{0(d)}(\varepsilon)$ expresses the effect of the interface potential $V^{0(d)}$ on the "free" Green function $G_0(\varepsilon)$, and $\Delta G^{0d}(\varepsilon)$ gives the contribution of the multiple reflections from both interfaces.

The density of states change $\Delta n(\varepsilon)$ responsible for the interlayer coupling is given by $\Delta G^{0d}(\varepsilon)$, Eq. (5), and therefore as it follows from Eq. (3),

$$\Delta n(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\mathrm{Tr}\langle\Delta G^{0d}(\varepsilon + i0^+)\rangle. \tag{6}$$

Using the definitions (5) for $G_0(\varepsilon)$ and $T^{0(d)}(\varepsilon)$, it may be shown that

$$\mathrm{Tr}\,\Delta G^{0d}(\varepsilon) = \frac{d}{d\varepsilon}\mathrm{Tr}\ln[1 - G_0(\varepsilon)T^0(\varepsilon)G_0(\varepsilon)T^d(\varepsilon)]. \tag{7}$$

Making use of Eqs. (6) and (7), the potential change (2) caused by the electron interferences in the spacer after integrating by parts may be represented as

$$\Delta\Phi = \frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty}d\varepsilon f(\varepsilon) \times\mathrm{Tr}\langle\ln[1 - G_0^+(\varepsilon)T^{0+}(\varepsilon)G_0^+(\varepsilon)T^{d+}(\varepsilon)]\rangle, \tag{8}$$

where $f(\varepsilon)$ is the Fermi-Dirac distribution and superscript + means that the energy ε has an infinitesimal imaginary part ($i0^+$).

Thus to get the interlayer coupling energy (8), one needs to have the "free" Green function in a spacer $G_0(\varepsilon)$ and to obtain the t-matrix $T^{0(d)}(\varepsilon)$ for a single interface located at $z=0$ or $z=d$, which according to Eq. (5) is defined by $G_0(\varepsilon)$ and perturbation $V^{0(d)}$ caused by the potential profile $U(z)$ and the random scatterers located at the interfaces (for disordered interfaces). In the framework of the adopted scattering formalism it is needed first to get the part of $V^{0(d)}$ due to the potential steplike profile $U(z)$.

A. Perfect interfaces

The goal of this section is to define the scattering matrix $T^{0(d)}$ caused by the potential steplike profile $U(z)$ for a single perfect interface which then will be generalized to the case of a disordered alloylike interface. We will use the approach of Ref. 19 but extended to the case when the electronic spectra of materials are treated in the EMA with different effective masses in different layers (in Ref. 19 the free electron spectra are used). For the case of material and spin dependent electron effective mass $m^*(z)$ and arbitrary conduction-band profile $U(z)$ (axis z is directed perpendicular to the interface) the Schrodinger equation for a single-electron state in the EMA reads

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*(z)}\nabla + U(z)\right]\Psi(x,y,z) = \varepsilon\Psi(x,y,z), \tag{9}$$

where $U(z)$ is a homogeneous potential taking different values at both sides of an interface [as well as $m^*(z)$]. By taking advantage of the two-dimensional homogeneity of the system [the in-plane wave vector $\mathbf{k}_\parallel=(k_x,k_y)$ is a good quantum number] and expanding the wave function in the complete set of the transverse wave functions $\phi_{\mathbf{k}_\parallel}(\rho)$,

$$\Psi(z,\rho) = \sum_{\mathbf{k}_\parallel}\psi_{\mathbf{k}_\parallel}(z)\phi_{\mathbf{k}_\parallel}(\rho), \quad \phi_{\mathbf{k}_\parallel}(\rho) = \frac{e^{i\mathbf{k}_\parallel\rho}}{\sqrt{A}}, \tag{10}$$

where $\rho=(x,y)$ is a two-dimensional vector in the plane of the interface and A is the area of the interface, Eq. (9) may be reduced to the following one-dimensional equation for the longitudinal wave function $\psi_{\mathbf{k}_\parallel}(z)$,

$$\left[\left(\frac{\partial}{\partial z}\right)\frac{1}{m^*(z)}\left(\frac{\partial}{\partial z}\right) + \frac{k^{\perp 2}(z;\varepsilon,\mathbf{k}_\parallel)}{m^*(z)}\right]\psi_{\mathbf{k}_\parallel}(z) = 0. \tag{11}$$

Here, the perpendicular wave vector $k^\perp(z;\varepsilon,\mathbf{k}_\parallel)$ is defined as

$$k^{\perp 2}(z;\varepsilon,\mathbf{k}_\parallel) = \frac{2m^*(z)}{\hbar^2}[\varepsilon - U(z)] - \mathbf{k}_\parallel^2. \tag{12}$$

Corresponding to Eq. (9), equation for the retarded Green function is

$$\left[\varepsilon + \frac{\hbar^2}{2}\nabla\frac{1}{m^*(z)}\nabla - U(z)\right]G^{z_0+}(\mathbf{r},\mathbf{r}';\varepsilon) = \delta(\mathbf{r} - \mathbf{r}'), \tag{13}$$

where the energy has an infinitesimal positive imaginary part and the index z_0 points out that the case of a single interface located at $z=z_0$ is being considered (for a trilayer $z_0=0$ or d). The Green function for the perfect interface and the δ function may be presented like Eq. (10) as

$$G^{z_0+}(\mathbf{r},\mathbf{r}';\varepsilon)=\frac{1}{A}\sum_{\mathbf{k}_\|} e^{i\mathbf{k}_\|(\rho-\rho')}G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\|),$$

$$\delta(\mathbf{r}-\mathbf{r}')=\frac{\delta(z-z')}{A}\sum_{\mathbf{k}_\|} e^{i\mathbf{k}_\|(\rho-\rho')}, \tag{14}$$

and Eq. (13) reduces to the one-dimensional equation for the Green function $G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\|)$,

$$\left[\left(\frac{\partial}{\partial z}\right)\frac{1}{m^*(z)}\left(\frac{\partial}{\partial z}\right)+\frac{k^{\perp 2}(z)}{m^*(z)}\right]G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\|)=\frac{2}{\hbar^2}\delta(z-z'). \tag{15}$$

This equation corresponds to the homogeneous Schrodinger equation (11).

The solution to Eq. (15) may be found in a standard way (see, e.g., Ref. 20) in terms of solutions to the Schrodinger equation (11) $\psi^L_{\mathbf{k}_\|}(z)$, $\psi^R_{\mathbf{k}_\|}(z)$, satisfying boundary conditions on the left and right sides, respectively. For the considered retarded Green function, $\psi^L_{\mathbf{k}_\|}(z)$ vanishes for $z\to-\infty$ and $\psi^R_{\mathbf{k}_\|}(z)$ vanishes for $z\to\infty$. This solution is

$$\begin{aligned}
G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\|)&=\frac{2}{\hbar^2}\frac{\psi^L(z)m^*(z')\psi^R(z')}{W(z')},\quad z<z',\\
G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\|)&=\frac{2}{\hbar^2}\frac{\psi^R(z)m^*(z')\psi^L(z')}{W(z')},\quad z>z',\\
W(z')&=\psi^L(z')\left[\frac{d\psi^R(z)}{dz}\right]_{z=z'}-\psi^R(z')\left[\frac{d\psi^L(z)}{dz}\right]_{z=z'},
\end{aligned} \tag{16}$$

where we omitted the index $\mathbf{k}_\|$ of the wave functions for brevity. The result given by Eq. (16) generalizes the corresponding formula of Ref. 19 to the case of different effective masses in different layers.

The solutions to Eq. (11) may be defined as

$$\begin{aligned}
\psi^L(z)&=\frac{1}{\sqrt{v_>}}e^{-ik_>(z-z_0)}+\frac{1}{\sqrt{v_>}}r_Le^{ik_>(z-z_0)},\quad z>z_0,\\
\psi^L(z)&=\frac{1}{\sqrt{v_<}}t_Le^{-ik_<(z-z_0)},\quad z<z_0,\\
\psi^R(z)&=\frac{1}{\sqrt{v_>}}t_Re^{ik_>(z-z_0)},\quad z>z_0,\\
\psi^R(z)&=\frac{1}{\sqrt{v_<}}e^{ik_<(z-z_0)}+\frac{1}{\sqrt{v_<}}r_Re^{-ik_<(z-z_0)},\quad z<z_0.
\end{aligned} \tag{17}$$

Here, $k_{>(<)}=\sqrt{\frac{2m_{>(<)}}{\hbar^2}[\varepsilon-U_{>(<)}]-\mathbf{k}_\|^2}$ is the perpendicular to the interface wave vector (12) taken to the right (left) of the interface situated at $z_0=0$ or $z_0=d$, $v_{>(<)}=\hbar k_{>(<)}/m_{>(<)}$, $m_{>(<)}$ and $U_{>(<)}$ are the electron effective mass $m^*(z)$ and potential $U(z)$ in the material to the right (left) side of the interface, and $r_{L(R)}$, $t_{L(R)}$ are the amplitudes of reflection from and transmission through the interface for an electron incoming to the interface from the right (left).

In order to obtain the reflection and transmission amplitudes one should match the wave functions (17) and their derivatives at the interface. Integration of Eq. (11) over z in a close vicinity of any interface results in the following continuity relations for derivatives:

$$\frac{1}{m_>}\left[\frac{d\psi^{L(R)}}{dz}\right]_{z_>}=\frac{1}{m_<}\left[\frac{d\psi^{L(R)}}{dz}\right]_{z_<}, \tag{18}$$

where $z_{>(<)}$ denotes the coordinate of the interface ($z=0$ or $z=d$) with an infinitesimal shift to the right (left). Then, the continuity relations for ψ^L, ψ^R and their derivatives result in

$$\begin{aligned}
&r_L=\frac{v_>-v_<}{v_>+v_<},\quad r_R=\frac{v_<-v_>}{v_>+v_<},\quad t_L=t_R=t=\frac{2\sqrt{v_>v_<}}{v_>+v_<},\\
&W_>=\frac{2im_>}{\hbar}t,\quad W_<=\frac{2im_<}{\hbar}t,
\end{aligned} \tag{19}$$

where $W_{>(<)}$ corresponds to $W(z')$ at z' taken to the right (left) side of the interface.

Substituting Eqs. (17) and (19) into Eq. (16), we get the following Green functions in different regions of z and z' (suppressing the arguments ε and $\mathbf{k}_\|$ for brevity):

$$\begin{aligned}
G^{z_0+}(z,z')&=\frac{1}{i\hbar\sqrt{v_>v_<}}te^{-ik_<(z-z_0)}e^{ik_>(z'-z_0)},\\
&\quad z<z_0,\quad z'>z_0,\\
G^{z_0+}(z,z')&=\frac{1}{i\hbar\sqrt{v_>v_<}}te^{ik_>(z-z_0)}e^{-ik_<(z'-z_0)},\\
&\quad z>z_0,\quad z'<z_0,\\
G^{z_0+}(z,z')&=\frac{1}{i\hbar v_<}[e^{ik_<|z-z'|}+r_Re^{-ik_<(z+z'-2z_0)}],\\
&\quad z<z_0,\quad z'<z_0,\\
G^{z_0+}(z,z')&=\frac{1}{i\hbar v_>}[e^{ik_>|z-z'|}+r_Le^{ik_>(z+z'-2z_0)}],\\
&\quad z>z_0,\quad z'>z_0.
\end{aligned} \tag{20}$$

Now, we can identify [in accordance with Eq. (5)] the "free" Green function (propagator) in the spacer sandwiched between interfaces located at $z_0=0$ and $z_0=d$. The last two lines of Eq. (20) represent the Green function for an electron incoming to a single interface from the left side (third line) and from the right side (fourth line). For the trilayer under consideration, we will adopt the following definitions for the material and spin dependent electron's effective mass and potential profile:

$$m^*(z) = m_1, \quad U(z) = U_1, \quad z < 0,$$

$$m^*(z) = m_2, \quad U(z) = U_2, \quad 0 < z < d,$$

$$m^*(z) = m_3, \quad U(z) = U_3, \quad z > d, \tag{21}$$

where indexes 1, 2, and 3 correspond to the layer at $z<0$, the spacer, and the layer at $z>d$, respectively. Thus for a "free" spacer electron incoming to the interfaces the corresponding propagator is

$$G_0^+(z,z';\varepsilon,\mathbf{k}_\parallel) = \frac{1}{i\hbar v_2} e^{ik_2|z-z'|}, \quad 0 \leqslant z, \quad z' \leqslant d, \tag{22}$$

where $v_i = \frac{\hbar k_i}{m_i}$ and $k_i = \sqrt{\frac{2m_i}{\hbar^2}(\varepsilon - U_i) - \mathbf{k}_\parallel^2}$ $(i=1,2,3)$. The contribution to the "free" propagator (22) due to the specular scattering from the perfect interface may be written as

$$\Delta G^0(z,z';\varepsilon,\mathbf{k}_\parallel) = \frac{1}{i\hbar v_2} r^0 e^{ik_2(z+z')},$$

$$\Delta G^d(z,z';\varepsilon,\mathbf{k}_\parallel) = \frac{1}{i\hbar v_2} r^d e^{-ik_2(z+z'-2d)},$$

$$0 < z, \quad z' < d, \tag{23}$$

where $\Delta G^{0(d)}$ is the contribution due to the scattering from the interface situated at $z=0(d)$ and $r^{0(d)}$ is the corresponding reflection amplitude from the left (right) interface [see Eq. (19)]

$$r^0 = \frac{v_2 - v_1}{v_1 + v_2}, \quad r^d = \frac{v_2 - v_3}{v_2 + v_3}. \tag{24}$$

On the other hand, by expanding $G(\mathbf{r},\mathbf{r}';\varepsilon)$, Eq. (14), into $V^0(z) = W^0\delta(z)$ or $V^d(z) = W^d\delta(z-d)$, where $W^{0(d)}$ is the potential (that we are looking for) responsible for specular reflection of an electron from a perfect interface located at $z=0(d)$, one gets [in accordance with Eq. (5)]

$$\Delta G^{0(d)}(z,z';\varepsilon,\mathbf{k}_\parallel) = \int dz_1 G_0(z,z_1;\varepsilon,\mathbf{k}_\parallel) \times T^{0(d)}(z_1;\varepsilon,\mathbf{k}_\parallel) G_0(z_1,z';\varepsilon,\mathbf{k}_\parallel), \tag{25}$$

where the t-scattering matrix is

$$T^0(z_1;\varepsilon,\mathbf{k}_\parallel) = T^0(\varepsilon,\mathbf{k}_\parallel)\delta(z_1),$$

$$T^0(\varepsilon,\mathbf{k}_\parallel) = \frac{W^0}{1 - G_0(0,0;\varepsilon,\mathbf{k}_\parallel)W^0},$$

$$T^d(z_1;\varepsilon,\mathbf{k}_\parallel) = T^d(\varepsilon,\mathbf{k}_\parallel)\delta(z_1 - d),$$

$$T^d(\varepsilon,\mathbf{k}_\parallel) = \frac{W^d}{1 - G_0(d,d;\varepsilon,\mathbf{k}_\parallel)W^d}. \tag{26}$$

Using Eq. (22), we have

$$T^{0+}(\varepsilon,\mathbf{k}_\parallel) = \frac{i\hbar v_2 W^0}{i\hbar v_2 - W^0}, \quad T^{d+}(\varepsilon,\mathbf{k}_\parallel) = \frac{i\hbar v_2 W^d}{i\hbar v_2 - W^d}. \tag{27}$$

Comparing Eq. (23) with Eq. (25) and using Eq. (22), we get

$$T^{0+}(\varepsilon,\mathbf{k}_\parallel) = i\hbar v_2 r^0, \quad T^{d+}(\varepsilon,\mathbf{k}_\parallel) = i\hbar v_2 r^d. \tag{28}$$

Finally, Eqs. (27), (28), and (24) yield

$$W^0 = \frac{i\hbar}{2}(v_2 - v_1), \quad W^d = \frac{i\hbar}{2}(v_2 - v_3), \tag{29}$$

where the potentials W^0 and W^d define the quantum reflection of a spacer electron from the left and right interface, respectively, and depend [according to Eq. (29)] on ε and $\mathbf{k}_\parallel$ (through the electron velocities).

Formulas (29) represent the main result of this section: we have managed to find the potential localized at the interface coordinate z_0,

$$V^{z_0}(z;\varepsilon,\mathbf{k}_\parallel) = W^{z_0}(\varepsilon,\mathbf{k}_\parallel)\delta(z - z_0), \tag{30}$$

which in the framework of the general scattering theory allows finding the reflection amplitude by calculating the t-scattering matrix (26) and then using Eq. (28).

Now, we can obtain an exact formula for the coupling energy (8) in the considered case of a trilayer with perfect interfaces. Making use of Eqs. (22) and (28) and taking a trace over z coordinates, we have

$$\Delta\Phi = \frac{1}{\pi} \operatorname{Im} \sum_{\mathbf{k}_\parallel} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \ln[1 - r^0 r^d e^{2ik_2 d}], \tag{31}$$

where r^0, r^d are defined by Eq. (24) and dependent on ε and $\mathbf{k}_\parallel$ (via the electron perpendicular velocities v_i, $i=1$, 2, and 3) as well as the perpendicular to the interfaces electron vector k_2 in a spacer. The symbol $\langle\cdots\rangle$ is absent for the case of perfect interfaces. The expression (31) was earlier obtained in a different way and analyzed in Ref. 8. Our derivation differs by using the EMA for electronic spectra (with different effective masses in different layers), but more importantly, we have obtained the potentials $V^{0(d)}$ [defined by Eqs. (29) and (30)], which in the adopted scattering theory approach describe the quantum reflections of electrons from the steplike potential $U(z)$. In addition to being interesting from the general quantum mechanical point of view, this will allow us to generalize the adopted approach and formula (31) to the case of disordered interfaces.

B. Disordered interfaces

In this section we will obtain the t-scattering matrix $T^{0(d)}$ for a single disordered interface needed for determining the coupling energy (8). In contrast to a perfect interface, the in-plane electron wave vector $\mathbf{k}_\parallel$ is no longer conserved. We will model the interfacial disorder by the short-range scattering centers located in the interfaces planes (x,y) and giving rise to the corresponding scattering potentials $V_i^{z_0}(\mathbf{r}) = V_i^{z_0}(\rho)\delta(z_0)$, where $\rho=(x,y)$ and $z_0(=0,d)$ is the position of the interface. Thus we will present the interfacial scattering potential $V^{0(d)}$ as a sum of the potential caused by the potential profile (30) and $V_i^{z_0}(\mathbf{r})$,

$$V^0(\rho,z) = [W^0 + V_i^0(\rho)]\delta(z),$$

$$V^d(\rho,z) = [W^d + V_i^d(\rho)]\delta(z-d). \tag{32}$$

It is useful to introduce the translationally invariant generally non-Hermitian single-site coherent potential σ^{z_0} defining the corresponding translationally invariant interfacial reference medium. Then, the interfacial scattering potential $V_i^{0(d)}(\rho)$ may be presented as

$$V_i^0(\rho) = \sum_{\alpha} (\sigma^0 + \tilde{\gamma}_\alpha^0)\delta(\rho - \rho_\alpha),$$

$$V_i^d(\rho) = \sum_{\alpha'} (\sigma^d + \tilde{\gamma}_{\alpha'}^d)\delta(\rho - \rho_{\alpha'}). \tag{33}$$

Here, a summation is over all randomly distributed δ scatterers located at the interfaces with the transverse positions ρ_α ($\rho_{\alpha'}$) and strengths $\gamma_\alpha^{0(d)} = \tilde{\gamma}_\alpha^{0(d)} + \sigma^{0(d)}$, where $\tilde{\gamma}_\alpha^{0(d)} = \gamma_\alpha^{0(d)} - \sigma^{0(d)}$. If disorder is present at the interface only [as it is assumed by Eq. (33)], then the values γ_α^0 can be estimated via the on-site potentials in the materials separated by the interface, i.e., $\gamma_\alpha^{0(d)} \sim (|U_< - U_>|/2)(a/2)^3$, where a is the lattice constant.

In the presence of the interface impurity potential $V_i^{0(d)}$ the reflection from the interface may in general be both specular (conserving $\mathbf{k}_\parallel$) and diffuse (not conserving $\mathbf{k}_\parallel$). It is convenient to describe these kinds of scatterings in the $\mathbf{k}_\parallel$ representation in which the diagonal in this representation t-matrix will define the specular scattering and the nondiagonal part of $T^{0(d)}(z;\varepsilon,\mathbf{k}_\parallel,\mathbf{k}_\parallel')$ will correspond to the diffuse scattering. The $\mathbf{k}_\parallel$ representation of the Green function describing the electron transport for the case of a single disordered interface situated at $z = z_0$ may be defined as [compare with Eq. (14)]

$$G^{z_0+}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{A}\sum_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} e^{i(\mathbf{k}_\parallel \rho - \mathbf{k}_\parallel' \rho')} G^{z_0+}(z,z';\varepsilon,\mathbf{k}_\parallel,\mathbf{k}_\parallel'). \tag{34}$$

To get the scattering t-matrix $T^{0(d)}(z;\varepsilon,\mathbf{k}_\parallel,\mathbf{k}_\parallel')$ for a spacer electron reflecting from a single interface, we will transform [with the help of Eq. (34)] the expansion of the Green function $G^{z_0+}(\mathbf{r},\mathbf{r}';\varepsilon)$ in the $\mathbf{r}$ representation (ε-dependence is suppressed),

$$\begin{aligned} G^{0(d)}(\mathbf{r},\mathbf{r}') &= G_0(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}_1 G_0(\mathbf{r},\mathbf{r}_1)V^{0(d)}(\mathbf{r}_1)G_0(\mathbf{r}_1,\mathbf{r}') \\ &\quad + \int d\mathbf{r}_1 \int d\mathbf{r}_2 G_0(\mathbf{r},\mathbf{r}_1)V^{0(d)}(\mathbf{r}_1)G_0(\mathbf{r}_1,\mathbf{r}_2) \\ &\quad \times V^{0(d)}(\mathbf{r}_2)G_0(\mathbf{r}_2,\mathbf{r}') + \cdots, \end{aligned} \tag{35}$$

into the expansion in $\mathbf{k}_\parallel$ representation,

$$\begin{aligned} G^{z_0}(z,z';\mathbf{k}_\parallel,\mathbf{k}_\parallel') &= G_0(z,z';\mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} + \int dz_1 G_0(z,z_1;\mathbf{k}_\parallel) \\ &\quad \times T^{z_0}(z_1;\mathbf{k}_\parallel,\mathbf{k}_\parallel')G_0(z_1,z';\mathbf{k}_\parallel'). \end{aligned} \tag{36}$$

Here, the scattering (from the interface) t-matrix in $\mathbf{k}_\parallel$ representation is defined as

$$T^{z_0}(z;\mathbf{k}_\parallel,\mathbf{k}_\parallel') = T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')\delta(z - z_0),$$

$$\begin{aligned} T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') &= [\tilde{W}^{z_0}(\mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} + \tilde{V}^{z_0}_{i\mathbf{k}_\parallel \mathbf{k}_\parallel'}] \\ &\quad + \sum_{\mathbf{k}_{1\parallel}} [\tilde{W}^{z_0}(\mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}_{1\parallel}} + \tilde{V}^{z_0}_{i\mathbf{k}_\parallel \mathbf{k}_{1\parallel}}] \\ &\quad \times G_0(z_0,z_0;\mathbf{k}_{1\parallel})[\tilde{W}^{z_0}(\mathbf{k}_{1\parallel})\delta_{\mathbf{k}_{1\parallel}\mathbf{k}_\parallel'} + \tilde{V}^{z_0}_{i\mathbf{k}_{1\parallel}\mathbf{k}_\parallel'}] + \cdots, \end{aligned} \tag{37}$$

where

$$\tilde{W}^{0(d)}(\mathbf{k}_\parallel) = W^{0(d)}(\mathbf{k}_\parallel) + n_i^{0(d)}\sigma^{0(d)},$$

$$\tilde{V}^{0(d)}_{i\mathbf{k}_\parallel \mathbf{k}_\parallel'} = \sum_{\alpha} (\tilde{V}_\alpha^{0(d)})_{\mathbf{k}_\parallel \mathbf{k}_\parallel'},$$

$$(\tilde{V}_\alpha^{0(d)})_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} = \frac{1}{A}\tilde{\gamma}_\alpha^{0(d)} e^{-i(\mathbf{k}_\parallel - \mathbf{k}_\parallel')\rho_\alpha}, \tag{38}$$

$n_i^{0(d)} = N_i^{0(d)}/A$ is the interface impurity density [$N_i^{0(d)}$ is the number of interfacial defects]. Scattering matrix $T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')$, Eq. (37), may be viewed as the matrix element $\langle \mathbf{k}_\parallel | \cdots | \mathbf{k}_\parallel' \rangle$ of the following operator:

$$\begin{aligned} T^{z_0} &= (\tilde{W}^{z_0} + \tilde{V}_i^{z_0})\frac{1}{(1 - G_0^{z_0}\tilde{W}^{z_0}) - G_0^{z_0}\tilde{V}_i^{z_0}} \\ &= (\tilde{W}^{z_0} + \tilde{V}_i^{z_0}) + (\tilde{W}^{z_0} + \tilde{V}_i^{z_0})G_0^{z_0}(\tilde{W}^{z_0} + \tilde{V}_i^{z_0}) \\ &\quad + (\tilde{W}^{z_0} + \tilde{V}_i^{z_0})G_0^{z_0}(\tilde{W}^{z_0} + \tilde{V}_i^{z_0})G_0^{z_0}(\tilde{W}^{z_0} + \tilde{V}_i^{z_0}) + \cdots, \end{aligned} \tag{39}$$

where the matrix elements of $\tilde{W}^{z_0}$ and $\tilde{V}_i^{z_0}$ are defined by Eqs. (37) and (38) and $G_0^{z_0}$ is the Green operator diagonal in the $\mathbf{k}_\parallel$ representation $\langle \mathbf{k}_\parallel | G_0^{z_0} | \mathbf{k}_\parallel' \rangle = G_0(z_0,z_0;\mathbf{k}_\parallel)\delta_{\mathbf{k}_\parallel \mathbf{k}_\parallel'} = \frac{1}{i\hbar v_2(\mathbf{k}_\parallel)}\delta_{\mathbf{k}_\parallel \mathbf{k}_\parallel'}$ [see Eq. (22) for the "free" electron propagator].

Using the identity for two arbitrary operators A and B

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}B\frac{1}{A+B}, \tag{40}$$

the series (39) may be rearranged as

$$\begin{aligned} T^{z_0} &= \tilde{W}^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}} + \frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}} \\ &\quad + \frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}}G_0^{z_0}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}} \\ &\quad + \frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}} \\ &\quad \times G_0^{z_0}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}}G_0^{z_0}\tilde{V}_i^{z_0}\frac{1}{1 - G_0^{z_0}\tilde{W}^{z_0}} + \cdots, \end{aligned} \tag{41}$$

where we have taken into account that $G_0^{z_0}$ and $\tilde{W}^{z_0}$ (both diagonal in $\mathbf{k}_\parallel$ representation) commute. It follows from Eqs.

(22), (29), and (38) that the first term of expansion (41), diagonal in $\mathbf{k}_\parallel$ representation, is equal to

$$\frac{\widetilde{W}^{z_0}(\mathbf{k}_\parallel)}{1 - G_0(z_0,z_0;\mathbf{k}_\parallel)\widetilde{W}^{z_0}(\mathbf{k}_\parallel)} = i\hbar v_2(\mathbf{k}_\parallel)\widetilde{r}^{\,z_0}(\mathbf{k}_\parallel), \tag{42}$$

where $\widetilde{r}^{\,z_0}(\mathbf{k}_\parallel)$ is the specular reflection amplitude from the "perfect" interface (located at $z_0=0$ or $z_0=d$) with the homogeneous effective potential σ^{z_0},

$$\widetilde{r}^0(\mathbf{k}_\parallel) = \frac{v_2 - v_1 - \dfrac{2i}{\hbar}\Sigma^0}{v_2 + v_1 + \dfrac{2i}{\hbar}\Sigma^0}, \quad \widetilde{r}^d(\mathbf{k}_\parallel) = \frac{v_2 - v_3 - \dfrac{2i}{\hbar}\Sigma^d}{v_2 + v_3 + \dfrac{2i}{\hbar}\Sigma^d}, \tag{43}$$

which was first obtained in Ref. 18, and $\Sigma^{z_0}=n_i^{z_0}\sigma^{z_0}$. Another factor entering Eq. (41) is

$$\frac{1}{1 - G_0(z_0,z_0;\mathbf{k}_\parallel)\widetilde{W}^{z_0}(\mathbf{k}_\parallel)} = i\hbar v_2(\mathbf{k}_\parallel)\widetilde{G}^{z_0+}(\mathbf{k}_\parallel). \tag{44}$$

Here, $\widetilde{G}^{z_0+}(\mathbf{k}_\parallel)$ is the effective-medium retarded Green function (propagator)

$$\widetilde{G}^{0+}(\mathbf{k}_\parallel) = \frac{2}{i\hbar\left(v_1 + v_2 + \dfrac{2i}{\hbar}\Sigma^0\right)},$$

$$\widetilde{G}^{d+}(\mathbf{k}_\parallel) = \frac{2}{i\hbar\left(v_2 + v_3 + \dfrac{2i}{\hbar}\Sigma^d\right)}, \tag{45}$$

defining (as it is shown in Ref. 18) the specular part of the transmission through the disordered interface (located at $z_0=0,d$) which is characterized by the effective potential Σ^{z_0}. In fact, the functions (45) are the $\mathbf{k}_\parallel$ representation of the Green function (34) for the case of "perfect" interfaces with a homogeneous effective potential Σ^{z_0} [compare with the first two lines of Eq. (20)]. The specular reflection [of a spacer electron with a velocity $v_2(\mathbf{k}_\parallel)$] amplitude (43) from such a "perfect" interface may also be expressed via functions (45) as

$$\widetilde{r}^{\,z_0}(\mathbf{k}_\parallel) = i\hbar v_2(\mathbf{k}_\parallel)\widetilde{G}^{z_0}(\mathbf{k}_\parallel) - 1. \tag{46}$$

On the other hand, the complete reflection amplitude $r^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')$ accounting for the electron specular and diffuse scattering of a spacer electron from the disordered interface may be expressed through the $\mathbf{k}_\parallel$ representation of the complete Green function (34), describing the electron propagation through a disordered interface, as[18]

$$r_i^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') = i\hbar\sqrt{v_2(\mathbf{k}_\parallel)v_2(\mathbf{k}_\parallel')}\,G^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') - \delta_{\mathbf{k}_\parallel\mathbf{k}_\parallel'}, \tag{47}$$

where

$$G^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') = \widetilde{G}^{z_0}(\mathbf{k}_\parallel)\,\delta_{\mathbf{k}_\parallel\mathbf{k}_\parallel'} + \widetilde{G}^{z_0}(\mathbf{k}_\parallel)T_i^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')\widetilde{G}^{z_0}(\mathbf{k}_\parallel'),$$

$$T_i^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') = \widetilde{V}^{z_0}_{i\mathbf{k}_\parallel\mathbf{k}_\parallel'} + \sum_{\mathbf{k}_{1\parallel}} \widetilde{V}^{z_0}_{i\mathbf{k}_\parallel\mathbf{k}_{1\parallel}}\widetilde{G}^{z_0}(\mathbf{k}_{1\parallel})\widetilde{V}^{z_0}_{i\mathbf{k}_{1\parallel}\mathbf{k}_\parallel'} + \cdots, \tag{48}$$

and $\widetilde{G}^{z_0}(\mathbf{k}_\parallel)$ is given by Eq. (45). The specular part of the reflection amplitude (47) is given by its diagonal part, Eq. (46), and the diffuse part is defined by the electron scattering on the potential fluctuations (from the effective-medium potential σ^{z_0}) $\widetilde{V}_i^{z_0}$.

Thus with accounting for Eqs. (41), (42), (44), and (46)–(48), $T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')$, Eq. (37), finally takes the form [compare with Eq. (28)]

$$T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel') = i\hbar\sqrt{v_2(\mathbf{k}_\parallel)v_2(\mathbf{k}_\parallel')}\,r_i^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel'). \tag{49}$$

Returning to the general formula (8) for the coupling energy caused by the multiple scattering of the spacer electrons from the disordered interfaces, we see that it may be found by making use of the expression (22) for the "free" electron propagator in a spacer and z-dependent t-scattering matrices $T^0(z;\mathbf{k}_\parallel,\mathbf{k}_\parallel')=T^0(\mathbf{k}_\parallel,\mathbf{k}_\parallel')\,\delta(z)$, $T^d(z;\mathbf{k}_\parallel,\mathbf{k}_\parallel')=T^d(\mathbf{k}_\parallel,\mathbf{k}_\parallel')\,\delta(z-d)$, where $T^{z_0}(\mathbf{k}_\parallel,\mathbf{k}_\parallel')$ is defined by Eq. (49) [the trace in Eq. (8) assumes the integrations over z variables]. As a result we have [compare with Eq. (31)]

$$\Delta\Phi = \frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)$$
$$\times\langle\mathbf{k}_\parallel|\langle\ln[1 - r_i^0(\varepsilon)e^{i\hat{k}_2 d}r_i^d(\varepsilon)e^{i\hat{k}_2 d}]\rangle|\mathbf{k}_\parallel\rangle, \tag{50}$$

where the matrix elements of the operators $r_i^{0(d)}$ are defined by Eq. (47), $\langle\mathbf{k}_\parallel|e^{i\hat{k}_2 d}|\mathbf{k}_\parallel'\rangle=e^{ik_2 d}\delta_{\mathbf{k}_\parallel\mathbf{k}_\parallel'}$ and $k_2=\sqrt{\frac{2m_2}{\hbar^2}(\varepsilon-U_2)-\mathbf{k}_\parallel^2}$ is the perpendicular to the interfaces component of the spacer electron wave vector.

Formula (50) is the main formal result of the paper which generalizes Eq. (31) to the case of disordered interfaces. It differs from Eq. (31) by averaging over all the arrangements of the mixed atoms at the disordered interfaces (inner brackets $\langle\cdots\rangle$) and by matrix elements of the reflection amplitudes $\langle\mathbf{k}_\parallel|r_i^{z_0}(\varepsilon)|\mathbf{k}_\parallel'\rangle$ which are generally nondiagonal and describe both the specular and diffuse scatterings. The averaging procedure applied in Eq. (50) to the logarithmic function is not generally an easy one to perform. It may be performed, for example, by expanding the logarithmic function and then taking the average of each term of this series expansion. In this paper, we will restrict ourselves to the first term of the logarithm expansion which is easiest for evaluation. At the same time, this is a good approximation (provides the main contribution) if the reflection amplitudes are small (small confinement in the spacer). The latter is the case, e.g., in the transition metal heterostructures, where the difference between on-site potentials in different layers (electronic band profile), which defines the intensity of both the quantum reflection from perfect interfaces and from defects located at the interfaces, is small as compared to the Fermi energy (for more details see below).

III. INTERLAYER EXCHANGE COUPLING

We now consider the small confinement case when $|r_i^0 r_i^d|$ is small. Then, the leading term of Eq. (50) is

$$\Delta\Phi = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\langle\langle\mathbf{k}_\parallel|r_i^0(\varepsilon)e^{i\hat{k}_2 d}r_i^d(\varepsilon)e^{i\hat{k}_2 d}|\mathbf{k}_\parallel\rangle\rangle. \tag{51}$$

The average over the scatterers configurations of the disordered interfaces integrand may be presented [with the help of Eqs. (47) and (48)] as

$$\begin{aligned}
&\langle\langle\mathbf{k}_\parallel|r_i^0(\varepsilon)e^{i\hat{k}_2 d}r_i^d(\varepsilon)e^{i\hat{k}_2 d}|\mathbf{k}_\parallel\rangle\rangle\\
&\quad= \{\tilde{r}^0(\mathbf{k}_\parallel)\tilde{r}^d(\mathbf{k}_\parallel) - i\hbar v_2(\mathbf{k}_\parallel)\tilde{G}^0(\mathbf{k}_\parallel)\langle T_i^0(\mathbf{k}_\parallel,\mathbf{k}_\parallel)\rangle\tilde{G}^0(\mathbf{k}_\parallel)\\
&\qquad - i\hbar v_2(\mathbf{k}_\parallel)\tilde{G}^d(\mathbf{k}_\parallel)\langle T_i^d(\mathbf{k}_\parallel,\mathbf{k}_\parallel)\rangle\tilde{G}^d(\mathbf{k}_\parallel)\\
&\qquad + [i\hbar v_2(\mathbf{k}_\parallel)]^2\tilde{G}^0(\mathbf{k}_\parallel)\langle T_i^0(\mathbf{k}_\parallel,\mathbf{k}_\parallel)\rangle\tilde{G}^0(\mathbf{k}_\parallel)\tilde{G}^d(\mathbf{k}_\parallel)\\
&\qquad + [i\hbar v_2(\mathbf{k}_\parallel)]^2\tilde{G}^d(\mathbf{k}_\parallel)\langle T_i^d(\mathbf{k}_\parallel,\mathbf{k}_\parallel)\rangle\tilde{G}^d(\mathbf{k}_\parallel)\tilde{G}^0(\mathbf{k}_\parallel)\}e^{2ik_2 d}\\
&\qquad + \sum_{\mathbf{k}'_\parallel}[i\hbar\sqrt{v_2(\mathbf{k}_\parallel)v_2(\mathbf{k}'_\parallel)}]^2\tilde{G}^0(\mathbf{k}_\parallel)\tilde{G}^0(\mathbf{k}'_\parallel)\tilde{G}^d(\mathbf{k}_\parallel)\tilde{G}^d(\mathbf{k}'_\parallel)\\
&\qquad \times\langle T_i^0(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)T_i^d(\mathbf{k}'_\parallel,\mathbf{k}_\parallel)\rangle e^{i(k_2+k'_2)d},
\end{aligned} \tag{52}$$

where $\tilde{G}^{0(d)}(\mathbf{k}_\parallel)$ and $\tilde{r}^{0(d)}(\mathbf{k}_\parallel)$ are given by Eqs. (45) and (46), respectively.

As it has been shown in Ref. 18 the specular scattering from a disordered interface (located at $z=z_0$) may be completely described by the Green function (45) for the effective (reference) medium Σ^{z_0} if we choose the coherent potential Σ^{z_0} in such a way that the averaged diagonal element of the t-scattering matrix satisfies the condition

$$\langle T_i^{z_0+}(\Sigma^{z_0+},\mathbf{k}_\parallel,\mathbf{k}_\parallel)\rangle = 0, \tag{53}$$

where the superscript + refers to the fact that we selected the retarded Green functions for the present consideration. Equation (53) determines the conventional coherent potential approximation (CPA) in the theory of disordered systems. We see from Eq. (52) that in this approximation the contribution of the specular reflections from the interfaces to the coupling energy (51) is completely defined by the specular reflection amplitudes $\tilde{r}^{z_0}(\mathbf{k}_\parallel)$ from an interface with translationally invariant impurity potential $\Sigma^{z_0+}=n_i^{z_0}\sigma^{z_0+}$ [thus we defined the non-Hermitian potential in Eq. (33) as σ^{z_0+}]. The last term in Eq. (52) describes the double scattering of electrons from the interfaces with nonconserving $\mathbf{k}_\parallel$ (diffuse scattering).

It is necessary to define more explicitly the coherent potential Σ^{z_0+} fixed by Eq. (53). Since we defined σ^{z_0+} as a single-site translationally invariant potential (independent of the site α and $\mathbf{k}_\parallel$), the self-consistency condition (53) should also be considered in the single-site approximation, i.e., $T_i^{z_0+}$ in this equation should be replaced with the t-scattering matrix in the single-site approximation.

The scattering t-matrix $T_i^{z_0}$, Eq. (48), in the operator form may be represented in terms of a single-site scattering t-matrix $t_\alpha^{z_0}$ as (see, e.g., Ref. 20)

$$\begin{aligned}
T_i^{z_0+} &= \sum_\alpha t_\alpha^{z_0+} + \sum_\alpha t_\alpha^{z_0+}\tilde{G}^{z_0+}\sum_{\beta\neq\alpha} t_\beta^{z_0+}\\
&\quad + \sum_\alpha t_\alpha^{z_0+}\tilde{G}^{z_0+}\sum_{\beta\neq\alpha} t_\beta^{z_0+}\tilde{G}^{z_0+}\sum_{\gamma\neq\beta} t_\gamma^{z_0+} + \cdots,
\end{aligned} \tag{54}$$

where the single-site scattering operator is

$$\begin{aligned}
t_\alpha^{z_0+} &= \tilde{V}_\alpha^{z_0} + \tilde{V}_\alpha^{z_0}\tilde{G}^{z_0+}\tilde{V}_\alpha^{z_0} + \tilde{V}_\alpha^{z_0}\tilde{G}^{z_0+}\tilde{V}_\alpha^{z_0}\tilde{G}^{z_0+}\tilde{V}_\alpha^{z_0} + \cdots\\
&= (1-\tilde{V}_\alpha^{z_0}\tilde{G}^{z_0+})^{-1}\tilde{V}_\alpha^{z_0}.
\end{aligned} \tag{55}$$

Here, the matrix elements of $\tilde{V}_\alpha^{z_0}$ and $\tilde{G}^{z_0+}$ are given by Eqs. (38) and (45), respectively.

Thus the matrix element of the scattering matrix (54) in the single-site approximation is

$$T_i^{z_0+}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel) = \sum_\alpha t_\alpha^{z_0+}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel),$$

$$t_\alpha^{z_0+}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel) = \frac{1}{A}\frac{\gamma_\alpha^{z_0}-\sigma^{z_0}}{1-(\gamma_\alpha^{z_0}-\sigma^{z_0})\frac{1}{A}\sum_{\mathbf{k}_{\parallel 1}}\tilde{G}^{z_0+}(\mathbf{k}_{\parallel 1})}e^{-i(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)\rho_\alpha}, \tag{56}$$

where a two-dimensional vector ρ_α specifies the positions of scatterers at the disordered interface [see Eq. (33)]. The average over scatterers' configuration $\langle t_\alpha^{z_0+}(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)\rangle$ is diagonal in $\mathbf{k}_\parallel$ space, equal to $t_\alpha^{z_0+}(\mathbf{k}_\parallel,\mathbf{k}_\parallel)$, and therefore does not depend on the positions of imperfections ρ_α. It may be seen explicitly if we adopt, e.g., the following configuration average procedure:

$$\langle f(\rho_1,\ldots,\rho_N)\rangle = \left[\prod_{\alpha=1}^{N_i}\int\frac{d\rho_\alpha}{A}\right]f(\rho_1,\ldots,\rho_{N_i}), \tag{57}$$

where $f(\rho_1,\ldots,\rho_{N_i})$ is some function of the scatterers coordinates. Then, Eq. (53) for the coherent potential Σ^{z_0+} reads

$$\sum_\alpha\frac{\gamma_\alpha^{z_0}-\sigma^{z_0}}{1-(\gamma_\alpha^{z_0}-\sigma^{z_0})\frac{1}{A}\sum_{\mathbf{k}_\parallel}\tilde{G}^{z_0+}(\mathbf{k}_\parallel)} = 0. \tag{58}$$

Now, we can see that the last (diffuse) term in Eq. (52) is equal to zero because the average procedure should be applied to each interface independently [the positions of scattering centers at $z=0(\rho_\alpha)$ and $z=d(\rho_{\alpha'})$ cannot coincide] and therefore according to Eqs. (57) and (58)

$$\langle T_i^0(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)T_i^d(\mathbf{k}'_\parallel,\mathbf{k}_\parallel)\rangle = \langle T_i^0(\mathbf{k}_\parallel,\mathbf{k}'_\parallel)\rangle\langle T_i^d(\mathbf{k}'_\parallel,\mathbf{k}_\parallel)\rangle = 0 \tag{59}$$

in the adopted coherent potential approximation for electron scattering at disordered interfaces.

Thus the coupling energy (51) takes the following form:

$$\Delta\Phi = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\tilde{r}^0(\mathbf{k}_\parallel)\tilde{r}^d(\mathbf{k}_\parallel)e^{2ik_2 d} \tag{60}$$

and is defined completely by the specular reflection amplitudes from disordered interfaces (43). It should be stressed, however, that these amplitudes are affected by diffuse scattering (see below).

Formula (60), obtained for the case of small reflection amplitudes, provides a relatively simple starting point for further consideration. It accounts for interference between an incident wave and a reflected wave resulting from only one round trip of an electron in the spacer and thus neglects the interference effects of the higher order originated from $n > 1$ round trips ($2n$ reflections from interfaces). Use of the single-site CPA (58) implies neglecting of scattering by clusters of defects at each interface, which is reasonable for the considered small scattering case assuming weak scattering by interfacial disorder also. The latter also means that the coherent potential, defined by Eq. (58), should be taken in the the weak scattering limit [see Eq. (79) and comments below]. Restriction to only one round trip of an electron in the spacer also results in neglecting the correlation effects between scatterings by defects occurring when an electron strikes the same disordered interface more than once (these effects arise in the next terms of the logarithm expansion in the small reflection amplitudes).

Expression (60) is valid for arbitrary materials making up the trilayer. We will now consider the case of a paramagnetic spacer (metallic or insulator) sandwiched between two ferromagnetic films. The quantum interferences of the electronic waves in the spacer induce an interlayer interaction between the ferromagnetic layers. In the ferromagnetic configuration of the magnetic layers

$$\Delta\Phi_F = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)[\tilde{r}_\uparrow^0(\mathbf{k}_\parallel)\tilde{r}_\uparrow^d(\mathbf{k}_\parallel) + \tilde{r}_\downarrow^0(\mathbf{k}_\parallel)\tilde{r}_\downarrow^d(\mathbf{k}_\parallel)]e^{2ik_2 d}, \tag{61}$$

while in the antiferromagnetic configuration

$$\Delta\Phi_{AF} = -\frac{1}{\pi}\,\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)[\tilde{r}_\uparrow^0(\mathbf{k}_\parallel)\tilde{r}_\downarrow^d(\mathbf{k}_\parallel) + \tilde{r}_\downarrow^0(\mathbf{k}_\parallel)\tilde{r}_\uparrow^d(\mathbf{k}_\parallel)]e^{2ik_2 d}, \tag{62}$$

where $\tilde{r}^{z_0}_{\uparrow(\downarrow)}$ stands for the reflection amplitude of a spacer electron with the spin parallel (antiparallel) to the magnetization direction of the magnetic layer at the ferromagnet-paramagnet interface situated at $z=z_0$. Evidently, $\tilde{r}^{z_0}_\uparrow \neq \tilde{r}^{z_0}_\downarrow$.

Taking the difference of these two expressions and replacing the sum over $\mathbf{k}_\parallel$ by the integral, we arrive at the following exchange coupling energy per unit interface area:

$$E_F - E_{AF} = -\frac{1}{\pi^3}\,\mathrm{Im}\int d\mathbf{k}_\parallel \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\Delta\tilde{r}^0(\mathbf{k}_\parallel)\Delta\tilde{r}^d(\mathbf{k}_\parallel)e^{2ik_2 d}, \tag{63}$$

where $E_F=\frac{\Delta\Phi_F}{A}$, $E_{AF}=\frac{\Delta\Phi_{AF}}{A}$, and the spin-dependent asymmetries of the reflection amplitudes

$$\Delta\tilde{r}^{z_0} = \frac{\tilde{r}^{z_0}_\uparrow - \tilde{r}^{z_0}_\downarrow}{2} \tag{64}$$

are introduced.

For simplicity, we take the ferromagnetic (semi-infinite) layers to be identical, i.e.,

$$\tilde{r}^0_{\uparrow(\downarrow)} = \tilde{r}^d_{\uparrow(\downarrow)} = \tilde{r}_{\uparrow(\downarrow)}, \quad \Delta\tilde{r}^0 = \Delta\tilde{r}^d = \Delta\tilde{r}. \tag{65}$$

According to Eq. (43), the reflection amplitudes from ferromagnetic layers may be defined as

$$\tilde{r}_{\uparrow(\downarrow)} = \frac{v_2 - v_{\uparrow(\downarrow)} - i\Gamma^+_{\uparrow(\downarrow)}}{v_2 + v_{\uparrow(\downarrow)} + i\Gamma^+_{\uparrow(\downarrow)}}. \tag{66}$$

Here, v_2 is the spacer electron velocity perpendicular to an interface,

$$v_2 = \frac{\hbar k_2}{m_2}, \quad \frac{\hbar^2 k_2^2}{2m_2} = \varepsilon + i0^+ - \frac{\hbar^2\mathbf{k}_\parallel^2}{2m_2} - U_2, \tag{67}$$

$v_{\uparrow(\downarrow)}$ is the electron perpendicular velocity in the ferromagnetic layer with the spin parallel (antiparallel) to the magnetization direction

$$v_{\uparrow(\downarrow)} = \frac{\hbar k_{\uparrow(\downarrow)}}{m_{\uparrow(\downarrow)}}, \quad \frac{\hbar^2 k_\uparrow^2}{2m_\uparrow} = \varepsilon + i0^+ - \frac{\hbar^2\mathbf{k}_\parallel^2}{2m_\uparrow},$$

$$\frac{\hbar^2 k_\downarrow^2}{2m_\downarrow} = \varepsilon + i0^+ - \frac{\hbar^2\mathbf{k}_\parallel^2}{2m_\downarrow} - \Delta, \tag{68}$$

Δ is the exchange split of spectrum in the ferromagnet, and

$$\Gamma^+_{\uparrow(\downarrow)} = \frac{2}{\hbar}\Sigma^+_{\uparrow(\downarrow)} = \frac{2}{\hbar}n_i\sigma^+_{\uparrow(\downarrow)} \tag{69}$$

is defined by a coherent potential of an intermixed ferromagnet-paramagnet interface (dependent generally of an electron energy ε) which is "felt" by a spacer electron with the spin parallel (antiparallel) orientation relative to the ferromagnet magnetization direction. Note that the effective masses of spin-up and spin-down electrons $m_{\uparrow(\downarrow)}$ are generally different and the condition (65) and the definition (69) imply that the intermixing of atoms at both ferromagnet-paramagnet interfaces are identical, i.e., $\Sigma^{0+}_{\uparrow(\downarrow)}=\Sigma^{d+}_{\uparrow(\downarrow)}=\Sigma^+_{\uparrow(\downarrow)}$.

As it follows from Eqs. (66)–(68), the reflection amplitudes depend on the perpendicular to the interfaces components of electron velocity (wave vector), which, of course, depend on the electron energy ε and the parallel to the interfaces component of the wave vector $\mathbf{k}_\parallel$ [see Eqs. (67) and (68)]. It is convenient to replace integration in Eq. (63) over ε and $\mathbf{k}_\parallel$ by integration over $\varepsilon_2=\frac{\hbar^2 k_2^2}{2m_2}+U_2$ and $\mathbf{k}_\parallel$, which may now be viewed as the independent variables of integration (see Ref. 8). Then, after integration over $\mathbf{k}_\parallel$ the exchange coupling energy (63) takes the form

$$E_F - E_{AF} = -\frac{2m_2}{\pi^2\hbar^2}k_B T\,\mathrm{Im}\int_{-\infty}^{\infty} d\varepsilon_2 (\Delta\tilde{r})^2 e^{2ik_2 d} \times \ln\left[1 + \exp\left(\frac{\varepsilon_F - \varepsilon_2}{k_B T}\right)\right], \tag{70}$$

where $\Delta\tilde{r}$ (as well as k_2) depends only on ε_2 (we assume that the effective mass of a spacer electron is close to the electron masses in the ferromagnet, i.e., $\frac{|m_2-m_{\uparrow(\downarrow)}|}{m_2+m_{\uparrow(\downarrow)}} \ll 1$). The integral

(70) may easily be evaluated at large spacer thickness d when the most important contribution to the coupling energy comes from the neighborhood of the Fermi energy ε_F (due to the rapidly varying exponential factor $e^{2ik_2 d}$). By expanding the exponential factor near ε_F and performing the change of variable

$$x = \exp\left(\frac{\varepsilon_F - \varepsilon_2}{k_B T}\right), \tag{71}$$

the integral (70) may be reduced to the tabulated integral (see also Ref. 8). The final result is

$$E_F - E_{AF} = (E_F - E_{AF})_{T=0} \frac{2\pi k_B T d/\hbar v^F}{\sinh(2\pi k_B T d/\hbar v^F)}, \tag{72}$$

where

$$(E_F - E_{AF})_{T=0} = \frac{m_2 v^{F2}}{2\pi^2 d^2} \operatorname{Im}[(\Delta\tilde{r}_F)^2 e^{2ik^F d}] \tag{73}$$

is the exchange coupling energy at zero temperature,

$$v^F = \frac{hk^F}{m_2}, \quad k^F = \sqrt{\frac{2m_2}{\hbar^2}(\varepsilon_F - U_2)} \tag{74}$$

is the Fermi velocity and wave vector for a spacer, $\Delta\tilde{r}_F$ is defined as

$$\Delta\tilde{r}_F = \frac{\tilde{r}^F_\uparrow - \tilde{r}^F_\downarrow}{2}, \quad \tilde{r}^F_{\uparrow(\downarrow)} = \frac{v^F - v^F_{\uparrow(\downarrow)} - i\Gamma^{+F}_{\uparrow(\downarrow)}}{v^F + v^F_{\uparrow(\downarrow)} + i\Gamma^{+F}_{\uparrow(\downarrow)}},$$

$$v^F_\uparrow = \frac{\hbar}{m_\uparrow}\sqrt{\frac{2m_\uparrow}{\hbar^2}\varepsilon_F}, \quad v^F_\downarrow = \frac{\hbar}{m\downarrow}\sqrt{\frac{2m_\downarrow}{\hbar^2}(\varepsilon_F - \Delta)}, \tag{75}$$

and $\Gamma^{+F}_{\uparrow(\downarrow)}$ denotes the coherent potential (69) taken at ε_F. For a metallic spacer $\varepsilon_F > U_2$ and $v^F(k^F)$ is real, while for an insulating spacer $\varepsilon_F < U_2$ and $v^F(k^F)$ is imaginary. It should be added that the integral (70) converges and the result (72) is only valid for

$$k_B T < \frac{1}{\operatorname{Im}\left(\frac{2d}{\hbar v^F}\right)}, \tag{76}$$

which imposes no restriction for a metallic spacer but restricts temperatures to the sufficiently low ones in the case of an insulating spacer.

The result given by Eqs. (72) and (73) differs from the one obtained in Refs. 11 and 8 by substitution $\Delta r_F = (r^F_\uparrow - r^F_\downarrow)/2$, where $r^F_{\uparrow(\downarrow)} = [v^F - v^F_{\uparrow(\downarrow)}]/[v^F + v^F_{\uparrow(\downarrow)}]$ is the spin-dependent reflection amplitude for a perfect interface, with the $\Delta\tilde{r}_F$, Eq. (75), defined for the disordered interface. This difference is very substantial because the coherent potential $\Gamma^F_{\uparrow(\downarrow)}$ is a complex quantity, i.e., $\Gamma^F_{\uparrow(\downarrow)} = \operatorname{Re}\Gamma^F_{\uparrow(\downarrow)} + i\operatorname{Im}\Gamma^F_{\uparrow(\downarrow)}$ (see Ref. 18 and below). The first consequence of this fact is that the real part of $\Gamma^F_{\uparrow(\downarrow)}$ leads to the emergence (for a metallic spacer) of the cosinelike oscillation of the interlayer coupling (73) in addition to the conventional sinelike behavior observed for perfect interfaces (when Δr_F is real). The temperature dependence of the interlayer coupling (72) is the same as for the case of perfect interfaces: the coupling decreases with temperature for a metallic spacer and increases with T in the case of an insulating spacer (see Ref. 8).

Since the self-energy (coherent potential) plays an important role in our calculations, we will now consider it in more detail. In Eq. (58) for a binary-alloy-type interface with atoms of type 1 (ferromagnetic atoms) and of type 2 (spacer atoms) intermixed, $\gamma_\alpha = \gamma_1, \gamma_2$, where $\gamma_1 = \gamma_{\uparrow(\downarrow)}$ is the strength of scattering of a spacer electron [with the spin parallel (antiparallel) to magnetization of the interface ferromagnet] by magnetic atoms, and γ_2 is the strength of scattering by the nonmagnetic atoms. Equation (58) may be rewritten, suppressing the interface index z_0, as follows:

$$\sigma_{\uparrow(\downarrow)} = \frac{\bar{\gamma}_{\uparrow(\downarrow)} - \gamma_{\uparrow(\downarrow)}\gamma_2 \frac{1}{A}\sum_{\mathbf{k}_\parallel} \tilde{G}^+_{\uparrow(\downarrow)}(\mathbf{k}_\parallel)}{1 - [\gamma_{\uparrow(\downarrow)} + \gamma_2 - \sigma_{\uparrow(\downarrow)}]\frac{1}{A}\sum_{\mathbf{k}_\parallel} \tilde{G}^+_{\uparrow(\downarrow)}(\mathbf{k}_\parallel)}, \tag{77}$$

where $\bar{\gamma}_{\uparrow(\downarrow)} = 1/N_i \Sigma_\alpha \gamma_\alpha = [c_1\gamma_{\uparrow(\downarrow)} + c_2\gamma_2]$ is the average strength of the interface scatterers due to disorder, $c_{1,2} = N_{1,2}/N_i$ are concentrations of the first (ferromagnetic) and second (nonmagnetic) materials mixed at the interface ($c_1 + c_2 = 1$). The strength of scatterers may be estimated via the difference of the one-site potentials for electrons at both sides of the interface. For a spacer electron $\gamma_\uparrow \sim U_2 a^3$, $\gamma_\downarrow \sim |U_2 - \Delta| a^3$, and $\gamma_2 = 0$, where we have used the model spectra (68). The effective-medium Green function $\tilde{G}^+(\mathbf{k}_\parallel)$ in Eq. (77) is defined by Eq. (45),

$$\tilde{G}^+_{\uparrow(\downarrow)}(\mathbf{k}_\parallel) = \frac{2}{i\hbar[v_{\uparrow(\downarrow)} + v_2 + i\Gamma^+_{\uparrow(\downarrow)}]}, \tag{78}$$

where $v_{\uparrow(\downarrow)}$ and v_2 are defined by Eqs. (67) and (68) (taken at $\varepsilon = \varepsilon_F$), respectively, and summation (integration) over the parallel to interface wave vector includes both propagating and evanescent intermediate states. The evanescent states come from integration over $k_\parallel > \min(k^F, k^F_{\uparrow(\downarrow)})$, where k^F is defined by Eq. (74), $k^F_\uparrow = \sqrt{\frac{2m_\uparrow}{\hbar^2}\varepsilon_F}$, $k^F_\downarrow = \sqrt{\frac{2m_\downarrow}{\hbar^2}(\varepsilon_F - \Delta)}$, $k^F_\uparrow > k^F_\downarrow, k^F$, and one of the electron velocities is purely imaginary. The summation in Eq. (77) over evanescent states should be cutoff at a wave vector $\alpha \min(k^F, k^F_{\uparrow(\downarrow)})$ ($\alpha > 1$) to account for the finite range of the scattering potential and to avoid an ultraviolet divergence which is a consequence of using the δ-like impurity potentials (33).

If $\bar{\gamma}_{\uparrow(\downarrow)} \neq 0$, the expression for the coherent potential $\sigma_{\uparrow(\downarrow)}$ may be obtained by iterating Eq. (77) using the small parameter $|\frac{2}{\hbar}\Sigma^+_{\uparrow(\downarrow)}|/v^F_{\uparrow(\downarrow)} \ll 1$ (weak scattering). Actually, for consistency of the adopted approximation (small reflection amplitudes) we should take the coherent potential in the lowest approximation in this weak scattering parameter. In the first approximation, $\sigma_{\uparrow(\downarrow)} = \bar{\gamma}_{\uparrow(\downarrow)}$, and therefore $\Sigma^+_{\uparrow(\downarrow)} = \operatorname{Re}\Sigma^+_{\uparrow(\downarrow)} = n_i\bar{\gamma}_{\uparrow(\downarrow)}$. In this approximation $\operatorname{Im}\Sigma^+_{\uparrow(\downarrow)} = 0$, which means that the electron diffuse scattering at a disordered interface, defined by the imaginary part of the coherent potential,[18] is absent. In the next approximation

$$\Sigma^{+}_{\uparrow(\downarrow)} = n_i \bar{\gamma}_{\uparrow(\downarrow)} + n_i[\overline{\gamma^2_{\uparrow(\downarrow)}} - \bar{\gamma}^2_{\uparrow(\downarrow)}]\frac{1}{A}\sum_{\mathbf{k}_\parallel} \tilde{G}^{+}_{\uparrow(\downarrow)}(\mathbf{k}_\parallel). \qquad (79)$$

Here, $\bar{\gamma}_{\uparrow(\downarrow)} = c_1\gamma_{\uparrow(\downarrow)}$, $\overline{\gamma^2_{\uparrow(\downarrow)}} = c_1\gamma^2_{\uparrow(\downarrow)}$ ($\gamma_2 = 0$), and $\tilde{G}^{+}_{\uparrow(\downarrow)}(\mathbf{k}_\parallel)$ is defined by Eq. (78), where $\Sigma^{+}_{\uparrow(\downarrow)}$ is substituted with $n_i\bar{\gamma}_{\uparrow(\downarrow)}$. The self-energy (coherent potential) is now complex as the second term in Eq. (79) has both the real and imaginary parts. In the case under consideration, the fluctuations of the scattering potential of the disordered interfaces, given by the second in Eq. (79), are small and therefore the real part of the scattering potential, contributing to the electron specular scattering at a disordered interface,[18] is much larger than the imaginary part. However, if we wish to take into account the diffuse scattering, the imaginary part of the coherent potential, given by the second term of Eq. (79), should be taken into consideration.

If $\bar{\gamma}_{\uparrow(\downarrow)} = 0$, then in the first approximation in the small parameter $|\frac{2}{\hbar}\Sigma^{+}_{\uparrow(\downarrow)}|/v^F_{\uparrow(\downarrow)}$, $\mathrm{Re}\,\Sigma^{+}_{\uparrow(\downarrow)} \sim \mathrm{Im}\,\Sigma^{+}_{\uparrow(\downarrow)}$, and $\mathrm{Re}\,\Sigma^{+}_{\uparrow(\downarrow)}$ is due to the contribution of evanescent states into the above-mentioned sum over $\mathbf{k}_\parallel$ (for more details see Refs. 21 and 18).

Equations (72)–(77) solve, under the accepted approximations, the problem of the interlayer exchange coupling in multilayers with disordered interfaces. The key element stipulating this coupling, $\Delta\tilde{r}_F$, Eq. (75), may be rewritten as

$$\Delta\tilde{r}_F = v^F \frac{(\tilde{v}^F_\downarrow - \tilde{v}^F_\uparrow) + i(\mathrm{Re}\,\Gamma^{+F}_\downarrow - \mathrm{Re}\,\Gamma^{+F}_\uparrow)}{(v^F + \tilde{v}^F_\uparrow + i\,\mathrm{Re}\,\Gamma^{+F}_\uparrow)(v^F + \tilde{v}^F_\downarrow + i\,\mathrm{Re}\,\Gamma^{+F}_\downarrow)}, \qquad (80)$$

where $\tilde{v}^F_{\uparrow(\downarrow)} = v^F_{\uparrow(\downarrow)} - \mathrm{Im}\,\Gamma^{+F}_{\uparrow(\downarrow)}$. Using the analytical properties of retarded Green functions $\tilde{G}^{+}_{\uparrow(\downarrow)}(\mathbf{k}_\parallel)$, it may be shown that $\mathrm{Im}\,\Gamma^{+}_{\uparrow(\downarrow)} \leqslant 0$. The electron velocity difference $v^F_\uparrow - v^F_\downarrow$, defining the specular reflection amplitude at a perfect interface, is of the $\frac{1}{2}v^F_\uparrow\frac{\Delta}{\varepsilon_F}$ order (we assumed that $\frac{\Delta}{\varepsilon_F} \ll 1$, which is the case for the transition metal heterostructures and is in agreement with the adopted approximation of a small electron confinement in a spacer). As formula (80) shows, the contribution of the interfacial disorder, caused by the intermixing of magnetic and nonmagnetic atoms at an interface, is defined by the difference of the interface coherent potential for spin-up and spin-down electrons $\Gamma^{+F}_\uparrow - \Gamma^{+F}_\downarrow$, i.e., by asymmetry of spin-dependent scattering due to the interfacial disorder. It follows from the above estimates that $|\Gamma^{+F}_\uparrow - \Gamma^{+F}_\downarrow| \sim \frac{1}{\hbar}n_i c_1\Delta a^3 = \frac{1}{\hbar}\frac{N_1}{A}\Delta a^3 = \frac{1}{\hbar}c_1 a\Delta$, where $\frac{N_1}{A}$ is the density of magnetic atoms at the mixed interface. Thus the relative contribution of an interface disorder $|\Gamma^{+F}_\uparrow - \Gamma^{+F}_\downarrow|/|v^F_\uparrow - v^F_\downarrow| \sim c_1 a k^F_\uparrow$. Evidently, when the concentration of magnetic atoms at a mixed interface goes to zero, the interface becomes perfect, i.e., made up from the nonmagnetic atoms only, and the contribution of interfacial disorder vanishes. On the other hand, when $c_1 \to 1$, the interface also tends to the perfect one but made up from the magnetic atoms only and the contribution of disorder should also vanish. Then, one may expect that the relative contribution of atoms' mixing at an interface to the exchange coupling would depend on the concentration of defects as $|\Gamma^{+F}_\uparrow - \Gamma^{+F}_\downarrow|/|v^F_\uparrow - v^F_\downarrow| = |\alpha| \sim c_1(1-c_1)ak^F_\uparrow$. Taking into account the complexity of the interface alloying process during fabrication of the multilayers and difficulties in controlling this process (see, e.g., Ref. 17), it seems reasonable to consider the parameter α as an adjustment parameter which may be evaluated experimentally. Anyway, one can see that the contribution of disorder to the interfacial coupling may be comparable with that of an electron confinement in a spacer.

It is convenient to introduce the dimensionless complex parameter

$$\alpha = \alpha' + i\alpha'' = [\mathrm{Re}(\Gamma^{+F}_\downarrow - \Gamma^{+F}_\uparrow) + i\,\mathrm{Im}(\Gamma^{+F}_\downarrow - \Gamma^{+F}_\uparrow)]/(v^F_\downarrow - v^F_\uparrow) \qquad (81)$$

and to rewrite Eq. (80) in terms of it. The result is

$$\Delta\tilde{r}_F = \frac{v^F(v^F_\downarrow - v^F_\uparrow)}{(v^F + \tilde{v}^F_\uparrow)(v^F + \tilde{v}^F_\downarrow)} \times \frac{[(1-\alpha'') + i\alpha']\left(1 - i\dfrac{\mathrm{Re}\,\Gamma^F_\uparrow}{v^F + \tilde{v}^F_\uparrow}\right)\left(1 - i\dfrac{\mathrm{Re}\,\Gamma^F_\downarrow}{v^F + \tilde{v}^F_\downarrow}\right)}{\left[1 + \left(\dfrac{\mathrm{Re}\,\Gamma^F_\uparrow}{v^F + \tilde{v}^F_\uparrow}\right)^2\right]\left[1 + \left(\dfrac{\mathrm{Re}\,\Gamma^F_\downarrow}{v^F + \tilde{v}^F_\downarrow}\right)^2\right]}. \qquad (82)$$

The real part of Eq. (81) α' describes the contribution of the specular scattering at disordered interfaces while the imaginary part α'' defines the contribution of the diffuse scattering. It is possible to simplify Eq. (82) in the case of small interfacial scattering, $|\Gamma^F_{\uparrow(\downarrow)}|/v^F_{\uparrow(\downarrow)} \ll 1$, using the following restrictions on the parameters α' and α'':

$$|\Gamma^F_{\uparrow(\downarrow)}|/|v^F + v^F_{\uparrow(\downarrow)}| \ll |\alpha'| \ll |1-\alpha''||v^F + v^F_{\uparrow(\downarrow)}|/|\Gamma^F_{\uparrow(\downarrow)}|. \qquad (83)$$

Then, the needed square of Eq. (82) takes the form

$$(\Delta\tilde{r}_F)^2 = (\Delta r_F)^2[(1-\alpha'')^2 - \alpha'^2 + 2i\alpha'(1-\alpha'')], \qquad (84)$$

where

$$\Delta r_F = \frac{v^F(v^F_\downarrow - v^F_\uparrow)}{(v^F + v^F_\uparrow)(v^F + v^F_\downarrow)} \qquad (85)$$

is the reflection amplitude difference $\Delta r_F = (r^F_\uparrow - r^F_\downarrow)/2$ for the perfect interface. Condition (83) implies that $|1-\alpha''|$ should not be too small, meaning that the diffuse scattering is not very prominent, and $|\alpha'|$, describing specular scattering, is not very small in the considered case of small interfacial scattering defined by the coherent potential $\Gamma^F_{\uparrow(\downarrow)}$. Particularly, condition (83) may be satisfied when fluctuations of the scattering potential are small ($|\alpha''| \ll 1$) and the electron scattering by disordered interface is caused mainly by the real part of $\Gamma^F_{\uparrow(\downarrow)}$ (average interface potential).

For the case of a metallic spacer, when v^F is real, the interlayer exchange coupling (73) with $(\Delta\tilde{r}_F)^2$ given by Eq. (84) may be represented as

$$(E_F - E_{AF})_{T=0} = \frac{m_2 v^{F^2} k^{F^2}}{2\pi^2}(\Delta r_F)^2 f(\alpha', \alpha''; k^F d),$$

$$f(\alpha',\alpha'';k^F d) = \frac{1}{(k^F d)^2}\{[(1-\alpha'')^2-\alpha'^2]\sin(2k^F d) + 2\alpha'(1-\alpha'')\cos(2k^F d)\}. \qquad (86)$$

Equation (86) shows that in the case of the disordered interfaces there are the conventional, existing at $\alpha=0$ when interfaces are perfect, sinelike term in the exchange coupling, and an additional cosinelike term, caused mainly by the real part of the parameter (81) (the real part of the interface coherent potential, responsible for the electron specular scattering by the interfacial disorder[18]). The behavior of Eq. (86), as a function of spacer thickness d, depends on the values of the parameters α' and α'' and their signs. Thus it can be expected that the experimental data on the interfacial exchange coupling in the real multilayers with disordered (alloylike) interfaces may by described, at least in the case of weak scattering, by the formula (86) with the properly selected fitting parameters α' and α''. As will be shown below, a similar expression for interfaces with different intermixings includes four fitting parameters.

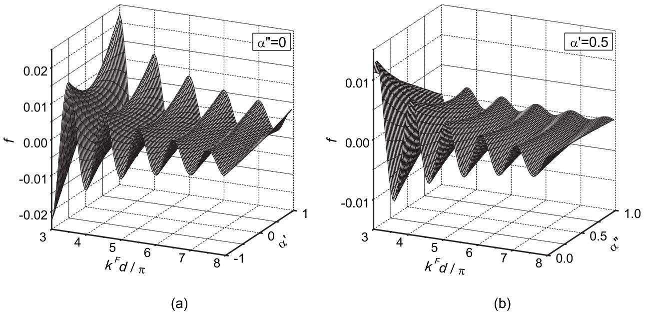
Let us qualitatively consider parameter α in more detail. It seems natural to relate $\Gamma_\uparrow^{+F}-\Gamma_\downarrow^{+F}$ to the spin-up-spin-down density of states difference at the Fermi energy ε_F. In the adopted EMA for the spectra of electrons, Eqs. (67) and (68), such a difference (per atom) is

$$\rho_\uparrow^F - \rho_\downarrow^F = \frac{a^3}{2\pi^2\hbar^3}\frac{m\Delta}{v_\uparrow^F}, \qquad (87)$$

where we assumed for simplicity that $m_\uparrow = m_\downarrow = m$ and $\frac{\Delta}{\varepsilon_F} \ll 1$. On the other hand, according to the simple estimate given above [for the case of weak scattering at interfacial disorder when the real part of $\Gamma_{\uparrow(\downarrow)}^F$ is given by the first term of Eq. (79)], $\mathrm{Re}(\Gamma_\uparrow^F-\Gamma_\downarrow^F) \sim c_1(1-c_1)a\Delta/\hbar$, i.e., this difference is defined by the spectrum exchange splitting in a ferromagnet as well as the density of state difference (87). Then, we may give the following estimate:

$$\mathrm{Re}(\Gamma_\uparrow^{+F}-\Gamma_\downarrow^{+F}) \sim \frac{2\pi^2\hbar^2 v_\uparrow^F}{a^2 m} c_1(1-c_1)(\rho_\uparrow^F-\rho_\downarrow^F). \qquad (88)$$

One can see from this very simplified consideration that the sign of the difference between the strengths of spin-up and spin-down electron scatterings at a disordered interface is naturally defined by the corresponding difference between their densities of states at the Fermi level. In the considered EMA, $\rho_\uparrow^F-\rho_\downarrow^F>0$, $v_\uparrow^F-v_\downarrow^F \approx \frac{1}{2}\frac{\Delta}{\varepsilon_F}>0$, and thus $\alpha'>0$; but, in many rather typical situations the spin-down electrons scatter more heavily, i.e., $\rho_\uparrow^F-\rho_\downarrow^F<0$ and α' may change sign. This follows from the fact that the EMA usually is not good, e.g., for spin-down electrons in such ferromagnets as Co, Ni, and Fe which are typically used for making magnetic multilayers exhibiting GMR (EMA may be good for the spin-up electrons in, e.g., Co and Ni, and for Cu electrons at the Fermi energy). Thus the parameter α' may generally have different signs. As to α'', from the physical point of view, it should be positive since the diffuse scattering at an interface may not increase the contribution to the interface coupling. These parameters may also have different values depending on the specific materials making up the multilayer. In the considered simple model we can see from Eqs. (87) and (88), and $v_\uparrow^F-v_\downarrow^F \approx \frac{1}{2}\frac{\Delta}{\varepsilon_F}$ that $\alpha' \sim c_1(1-c_1)k_\uparrow^F a$.



(a) (b)

FIG. 1. Interlayer coupling parameter f, Eq. (86), for two ferromagnetic layers separated by a nonmagnetic metallic spacer with disordered interfaces as a function of normalized spacer thickness and (a) specular scattering parameter α' for $\alpha''=0$ (no diffuse scattering), and (b) diffuse scattering parameter α'' for $\alpha'=1/2$. The surface grid is made up of lines of constant $k^F d$, and (a) α' or (b) α''. Note that in the adopted case of small scattering, valid values of α' and α'' are defined by conditions (83).

Equation (82) shows that at $|\alpha| \ll 1$ the influence of disorder on the interfacial coupling is small and the phase and amplitude of the coupling oscillations are almost the same as for the perfect interfaces. We will consider the situation when $|\alpha'|$ satisfies the condition (83), i.e., it is not too small (we have seen that this is possible and stipulated, e.g., by the average scattering potential of a disordered interface). When $|\alpha|$ grows, the scattering by disordered interfaces leads to a decrease of the conventional (existing at $\alpha=0$ when interfaces are perfect) sinelike term in the exchange coupling [first term in Eq. (86)] and to an emergence of the cosinelike term [$|1-\alpha''|$ is also not too small according to Eq. (83)]. The real part α', if large enough, may also change the sign of the sinelike term. Thus when $|\alpha|$ grows, the phase and amplitude of the dependence of exchange coupling oscillation on the spacer thickness change. Figure 1 illustrates dependencies of the dimensionless function f (86) on normalized spacer thickness and real and imaginary parts of the disordered interface scattering parameter α.

The amplitudes of both terms in Eq. (86) become equal when $|(1-\alpha'')^2-\alpha'^2| = 2|\alpha'(1-\alpha'')|$. When $\alpha'<0$ and the amplitudes of both terms in Eq. (86) become approximately equal, their superposition behaves as $\sqrt{2}\sin\!\left(2k^F d-\frac{\pi}{4}\right)$ or $-\sqrt{2}\cos\!\left(2k^F d-\frac{\pi}{4}\right)$ depending on the sign of the first term. For $\alpha'' \ll 1$, the former realizes when $\alpha' \approx -0.4$, and the latter when $\alpha' \approx -2.4$. Thus the cosine term leads to the oscillation phase shift which grows with $|\alpha'|$ reaching the value of $-\pi/4$ at $\alpha' \approx -0.4$, and further the value of $-3\pi/4$ at $\alpha' \approx -2.4$, when the sign of the first term in Eq. (86) becomes negative. It is also seen from Eq. (86) that the amplitude of oscillations grows with $|\alpha'|$. For $\alpha'>0$, the phase shift goes in the opposite direction (at given above values of $|\alpha'|$, the phase shifts are $\pi/4$ and $3\pi/4$, respectively). For $|\alpha'| = |1-\alpha''|$, the phase shift is $\pm\pi/2$ and the conventional $\sin(2k^F d)$ oscillations shift to the $\pm\cos(2k^F d)$ ones. When $\alpha'' \ll 1$, this realizes for $|\alpha'| \approx 1$ [see Fig. 1(a)]. As α'', which characterizes the diffuse scattering, grows, the amplitudes of both terms in Eq. (86) become smaller and the corresponding phase shifts are reached at smaller values of $|\alpha'|$. Thus larger diffuse scattering leads to larger phase shift (at the same value of α') and smaller oscillation amplitudes [see Fig. 1(b)]. The phase shift may reach π when $|\alpha'| \gg |1-\alpha''|$. Some experiments provide data for the phase shifts of the exchange coupling oscillations. For example, in Fe/Cr multilayers the phase of interface exchange oscillations was found to be opposite to that predicted theoretically.[22]

In reality, the intermixing of atoms at different interfaces are different, i.e., $\Sigma^{0+}_{\uparrow(\downarrow)} \neq \Sigma^{d+}_{\uparrow(\downarrow)}$ and, consequently, $\Delta\tilde{r}^{0} \neq \Delta\tilde{r}^{d}$. It is easy to generalize Eq. (86) to this case. The result is

$$(E_F - E_{AF})_{T=0} = \frac{m_2 v^{F2}}{2\pi^2 d^2}(\Delta r_F)^2\{[(1-\alpha''_0)(1-\alpha''_d) - \alpha'_0\alpha'_d] \times \sin(2k^F d) + [\alpha'_0(1-\alpha''_d) + \alpha'_d(1-\alpha''_0)]\cos(2k^F d)\}, \tag{89}$$

where the parameters $\alpha'_{0(d)}$ and $\alpha''_{0(d)}$ are the real and imaginary parts of the parameter $\alpha_{0(d)}$ defined as Eq. (81) for each interface located at $z=0$ and $z=d$, respectively. For validity of Eq. (89) these generally different parameters should satisfy condition (83) at each interface. Four parameters entering Eq. (89) provide more flexibility for adjusting the obtained expressions to the experiment.

IV. CONCLUSION

The theory of interlayer coupling in the nanostructures with the disordered alloylike interfaces is developed in the framework of the scattering theory based on the Green functions approach. We found it to be the most convenient formalism for treating the interlayer coupling through the basic mechanism of the electron waves interference resulting from multiple scattering of spacer electrons at both interfaces. This approach required reconsidering the specular electron reflection from a perfect interface in order to find the local potential responsible for such reflection. Conventionally, transmission through and reflection from an interface is considered by matching the electron wave functions and their derivatives at both sides of the interface. This approach becomes problematic for the interlayer coupling in the case of disordered interfaces when in addition to the specular scattering from a steplike potential, the diffuse scattering emerges and $\mathbf{k}_{\parallel}$ is not conserved. The obtained interface-localized potential responsible for the specular scattering at the perfect interface given by Eqs. (29) and (30) allows considering multiple scattering at potential steps (interfaces) in the framework of general scattering theory. This result also seems to be interesting from the general quantum mechanical point of view.

Using the local potential (29) and (30) due to the potential profile and adding the short-range potential (33) describing the interfacial scattering by a reference translationally invariant medium and the fluctuations of the scattering disorder potential, we obtained the general expression (50) for the interlayer coupling in the trilayer with disordered interfaces. In contrast to the similar expression for perfect interfaces (31) (see Ref. 8), expression (50) contains reflection amplitudes (47) for disordered interfaces (describing both the specular and diffuse scatterings) with averaging over all configurations of the atoms mixed at the interfaces. To get further analytical results, the small reflection amplitude case (small confinement) was considered, which is a good approximation for many practically important systems such as the transition metal based heterostructures [more complicated situations, when the next terms of the Eq. (50) expansion may be important, are planned to be considered]. In the single-site coherent potential approximation for the t-scattering matrix, the interlayer coupling (60) is obtained in terms of amplitudes of specular reflection Eq. (43) from the reference medium fixed by the CPA condition (53). This result was used to get the interlayer exchange coupling (72) between two ferromagnets divided by the nonmagnetic metal or insulator spacer. The contribution of disorder to this exchange coupling is defined by the difference of the interface coherent potential for spin-up and spin-down electrons $\Gamma^{+F}_{\uparrow} - \Gamma^{+F}_{\downarrow}$, i.e., by asymmetry of spin-dependent scattering due to the interfacial disorder [see Eq. (80)]. This contribution is described by the introduced dimensionless complex parameter α (81), which may be viewed as the adjustment parameter for relating the obtained expressions to experimental data. It has been estimated that the contribution of disorder to the interlayer coupling may be comparable with that of an electron confinement in a spacer with perfect interfaces and defined mainly by the real part of the complex coherent potential difference $\alpha' = \mathrm{Re}(\Gamma^{+F}_{\downarrow} - \Gamma^{+F}_{\uparrow})/(v^F_{\downarrow} - v^F_{\uparrow})$, which is related to the specular reflection from a disordered interface. This results in an emergence of a cosinelike term in addition to the conventional sinelike term in the exchange coupling for a metallic spacer. The primary effect of the superposition of these two terms is substantial, depending on the value of α, phase shift, and amplitude change in the oscillating exchange coupling in the GMR trilayer.

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