PHYSICAL REVIEW B, VOLUME 65, 214407

Crossover from diffusive to ballistic transport properties in magnetic multilayers

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(Received 7 January 2002; published 17 May 2002)

We develop a theoretical model for computing the spin-dependent transport properties of magnetic multilayers in the presence of ballistic scattering at the interfaces and diffusive scattering within the layers for currents perpendicular to the plane of the layers. The local chemical potentials are found to be momentum and spin dependent in the vicinity of regions with ballistic scattering. We have derived the approximate macroscopic equations from the Boltzmann equation by taking into account both ballistic and diffusive scattering. With these equations, realistic data of the reflection coefficients from *ab initio* calculations can be explicitly included in computing magnetotransport properties. We apply our formulation to a number of interesting magnetic multilayer structures.

DOI: 10.1103/PhysRevB.65.214407 PACS number(s): 75.70.Pa, 73.40.−c

I. INTRODUCTION

In the last decade, transport properties of mesoscopic systems have been extensively studied. Mesoscopic transport theories are now regarded as well established. For example, the Landauer-Buttiker formalism supplies a theoretical recipe to link the measured transport coefficients to microscopic transmission probabilities of a given mesoscopic system.[1] With existing transport theories, one does not have much difficulty in conceptually understanding important mesoscopic physics such as contact resistance,[2] conductance quanta and fluctuations,[3] and localization.[4]

In practice, however, one encounters difficulties in quantitatively calculating the conductance and magnetoresistance of a realistic experimental mesoscopic system. For example, let us consider a simple case where the conductor consists of two intimately contacted metallic magnetic layers with an interface at $z=0$. A current is applied perpendicular to the interface, and one measures the conductance by placing voltage probes far away from the interface. To correctly calculate the conductance, one has to introduce leads and reservoirs far away from the interface, and determine the transmission coefficients between the leads in the presence of interfacial and bulk impurity scattering. Such a calculation will be extremely tedious, if not entirely impossible, due to the vast numbers of conduction paths and scattering channels in the structure. Thus, instead of calculating the transmission coefficients of the whole structure, one usually calculates the transmission coefficient across a perfect interface by neglecting the bulk impurity scattering.[5] The effect of the bulk impurity is then added as an additional resistance. As already pointed out in a number of papers,[6–11] the resistance due to reflection at the interface depends on the bulk scattering in the layer. Thus the interface resistance calculated by neglecting the bulk scattering cannot be identified as the measured interface resistance.

The purpose of this paper is to establish an explicit expression for the transport property when the electron scattering is ballistic in one region and diffusive in another. We intend to develop a method to calculate the conductance and magnetoresistance by using the *ab initio* transmission coefficient as an input parameter. Our emphasis will be placed on relevant length scales involved in different scattering mechanisms. In Sec. II, we outline our model by defining the ballistic and diffusive transport with a specific model system. In Sec. III, we establish macroscopic transport equations for the transition region by using the semiclassical Boltzmann equation. Since there is intensive interest in magnetic multilayers, we will keep track of the spin dependence of the scattering, and will include spin relaxation processes. We solve these transport equations and calculate the conductance of the system using our well-defined boundary conditions. In particular, we show that the resistance is *not* a simple summation of the interface resistance and bulk resistance. Then we apply our theory to several interesting cases such as Co/Cu/Co and Fe/Au/Fe trilayers in Sec. IV. The detail derivation of the macroscopic transport equations are discussed in the Appendix.

II. MODEL

In this section, we first choose a model system which is simple enough to explicitly study the crossover from ballistic to diffusive transport. We consider two semi-infinite magnetic layers connected by an interface. A steady-state current flows perpendicular to the layers. The interface may have a finite thickness as long as the thickness is much smaller than the decoherence length of the conduction electrons. Thus applicable systems include spin valve structures of Co/Cu/Co and magnetic tunnel junctions of Co/Al_2O_2/Co. The conductance and magnetoresistance of this simple system were already presented in quite a few papers with different physical considerations; see the review articles in Refs. 12 and 13. The main difficulty in determining the conductance is that the Boltzmann equation in the presence of the specular reflection at the interface is not analytically solvable in general.[6–8,14–16] Instead, most of the theories simply neglect the spatial variation of the distribution function, and only focus on the effect of the electronic structure. Until recently, the interplay between diffusive scattering in the layers and ballistic scattering at interfaces has been emphasized.[17] Therefore, we intend to establish a connecting theory when the transport properties have both ballistic and diffusive components in the structure.

Before we proceed to evaluate the conductance of this system, let us first specify the length scales involved. The smallest length is the Fermi wavelength λ_F of the conduction electrons, of the order of the lattice constant for both spin-up and -down electrons. The next length scale is the electron mean free paths λ_s which characterize momentum relaxation in the layer. The longest transport length will be the spin diffusive length λ_{sf}. We will assume $\lambda_F \ll \lambda_s \ll \lambda_{sf}$ throughout the paper, so that the semiclassical Boltzmann equation is an adequate approach to describe the electron transport.[18]

For electrons near the interface (within the mean free path), the electrons travel across interface ballistically and thus the left- and right-going electrons have different energies. Strictly speaking, the electrons are hot, and the electrons do not satisfy the thermodynamic statistics. The concept of the local chemical potentials breaks down. Nevertheless, one can still introduce so-called "quasichemical potentials" to characterize the number of electrons at a given site.[19] In the presence of the current, the number of the left- and right-going electrons is different and one has to introduce a different chemical potential for left- and right-going electrons. Since the transmission coefficients depend on the spin for the magnetic interface, the chemical potential depends on the spin as well. Therefore, in the near-interface region, there are four chemical potentials for the left-going, right-going, spin-up, and spin-down electrons. In the intermediate region, i.e., when the electrons are a few mean free paths away from the interface but within the spin-diffusive length, the impurity scattering washes out the ballistic component of the electron transport. Thus the left- and right-going electrons merge into a common chemical potential. However, the spin-up and -down electrons continue to have different chemical potentials since the spin is not relaxed by non-spin-flip impurity scattering. Thus only two chemical potentials are required to describe the transport in the intermediate region. At the far region, i.e., when the electrons are away from the interface by a spin diffusion length, the transport becomes bulklike and one recovers the homogeneous bulk transport. There is no difference for spin-up and spin-down chemical potentials, i.e., only one chemical potential at a given location.

The above transport processes can be well described by using the Boltzmann equation with appropriate approximations. Within the relaxation-time approximation, there is no conceptual difficulty in writing down the Boltzmann equation. However, the solutions are difficult to obtain in the presence of the momentum dependence of the reflection coefficient at the interface.[6–8,14–17] As we show in the Appendix, the Boltzmann equation remains an integrodifferential equation even if one uses the relaxation-time approximation. When many attempts are made to numerically solve such an integrodifferential equation, a very limited physical insight into the interplay of the interface reflection and impurity scattering is gained. Here we revisit the Boltzmann equation, and derive a set of macroscopic equations using a plausible scheme to decouple the chemical potentials and current density in the distribution function, and thus the physical processes described in the preceding paragraph are shown explicitly.

III. MACROSCOPIC EQUATIONS

In this section, we outline the macroscopic equations used to calculate conductance and magnetoresistance. The derivation of these equations is given in the Appendix.

The macroscopic equations involve the spin-dependent current density and the local spin-dependent chemical potentials. In the layered structure, these macroscopic variables are translational invariant in the plane of the layers. Thus we label $\mu_s^{>}(z)$ as the chemical potential at position z (independent of x and y) for the electron with spin s (up or down) moving toward the right, i.e., $v_z > 0$. As we emphasized in Sec. II, the electrons are not necessary at the thermodynamic equilibrium if they are subject to ballistic scattering. Therefore, we need to keep track of the direction of the velocity in defining the chemical potential. Following the derivations from the Appendix, we find that the macroscopic equations for the chemical potentials, in the limit $\lambda_s \ll \lambda_{sf}$, are

$$\frac{d^2}{dz^2}(\mu_s^{>} - \mu_s^{<}) = \frac{\mu_s^{>} - \mu_s^{<}}{\lambda_s^2}, \tag{1}$$

$$\frac{d^2}{dz^2}(\overline{\mu}_s - \overline{\mu}_{-s}) = \frac{\overline{\mu}_s - \overline{\mu}_{-s}}{\lambda_{sf}^2} + \frac{\sqrt{3}}{4\lambda_s}\frac{d}{dz}(\mu_s^{>} - \mu_s^{<}) - \frac{\sqrt{3}}{4\lambda_{-s}}\frac{d}{dz}(\mu_{-s}^{>} - \mu_{-s}^{<}), \tag{2}$$

$$\frac{d^2}{dz^2}(\overline{\mu}_s + \overline{\mu}_{-s}) = \frac{P_s}{\lambda_{sf}^2}(\overline{\mu}_s - \overline{\mu}_{-s}) + \frac{\sqrt{3}}{4\lambda_s}\frac{d}{dz}(\mu_s^{>} - \mu_s^{<}) + \frac{\sqrt{3}}{4\lambda_{-s}}\frac{d}{dz}(\mu_{-s}^{>} - \mu_{-s}^{<}), \tag{3}$$

where λ_s is the mean free path projected to the z axis (and is equals $1/\sqrt{3}$ of the mean free path in three-dimensions; see the Appendix), λ_{sf} is the spin diffusion length, $P_s = (\rho_s - \rho_{-s})/(\rho_s + \rho_{-s})$ is the spin polarization of the ferromagnet (ρ_s is the resistivity), and we have defined $\overline{\mu}_s = (\mu_s^{>} + \mu_s^{<})/2$. The current density is related to these chemical potentials (see the Appendix)

$$j_s(z) = \frac{\sqrt{3}}{\rho_s}\left[-\frac{\partial \mu_s^{>}}{\partial z} - \frac{\partial \mu_s^{<}}{\partial z} + \frac{\sqrt{3}(\mu_s^{>} - \mu_s^{<})}{2\lambda_s} \right], \tag{4}$$

where $\rho_s = 6\pi^2\hbar/(e k_F^2 \lambda_s)$.

These macroscopic equations determine the diffusion properties of the conduction electrons: Eq. (1) characterizes the length scale of the hot electrons, i.e., it will take a length scale of the order of the mean free path to reach the thermodynamic equilibrium for the electrons scattered by the ballistic scattering at the interface; Eq. (2) describes the diffusion properties of the conduction electron spin, i.e., the chemical potentials of the electrons for different spin channels become identical after the electrons diffuse for a distance known as the spin-diffusion length. It is noted that the second and third terms on the right-hand side of Eq. (2) are absent in the ordinary spin-diffusion equation;[20,21] these terms come from the ballistic component of the interface scattering. Equation (3) governs the effects of these two diffusion processes on the average chemical potential which is ultimately related to the measured position dependence of the electric potential, and thereby determines the resistance and the magnetoresistance of the structure.

The solutions for each layer can be easily obtained from Eqs. (1)–(3). For example, for $z>0$, we have

$$\mu_s^{>}=\gamma_0+\gamma_1 z+\frac{C_1\lambda_{-s}}{\lambda_s+\lambda_{-s}}\exp\left(-\frac{z}{\lambda_{sf}}\right)+\alpha\left(1-\frac{\sqrt{3}}{2}\right)\exp\left(-\frac{z}{\lambda_s}\right), \tag{5}$$

$$\mu_s^{<}=\gamma_0+\gamma_1 z+\frac{C_1\lambda_{-s}}{\lambda_s+\lambda_{-s}}\exp\left(-\frac{z}{\lambda_{sf}}\right)-\alpha\left(1+\frac{\sqrt{3}}{2}\right)\exp\left(-\frac{z}{\lambda_s}\right), \tag{6}$$

$$\mu_{-s}^{>}=\gamma_0+\gamma_1 z-\frac{C_1\lambda_{s}}{\lambda_s+\lambda_{-s}}\exp\left(-\frac{z}{\lambda_{sf}}\right)+\beta\left(1-\frac{\sqrt{3}}{2}\right)\exp\left(-\frac{z}{\lambda_{-s}}\right), \tag{7}$$

$$\mu_{-s}^{<}=\gamma_0+\gamma_1 z-\frac{C_1\lambda_{s}}{\lambda_s+\lambda_{-s}}\exp\left(-\frac{z}{\lambda_{sf}}\right)-\beta\left(1+\frac{\sqrt{3}}{2}\right)\exp\left(-\frac{z}{\lambda_{-s}}\right). \tag{8}$$

Similar solutions can be written down for $z<0$ with the constants of integration γ_0, γ_1, C_1, α, and β replaced by γ_0', γ_1', C_1', α', and β', the exponential factors $\exp(-z/\lambda_s)$ and $\exp(-z/\lambda_{sf})$ are replaced by $\exp(z/\lambda_s)$ and $\exp(z/\lambda_{sf})$ to insure the decay solution as $z\rightarrow-\infty$, and $\sqrt{3}$ is changed to $-\sqrt{3}$. Clearly, the solution contains two characteristic decay lengths: the mean free path and the spin diffusion length. If there is no ballistic transmission and reflection at the interface, one would find that electron conduction is diffusive and one recovers Valet-Fert type of the equation when there is no difference between $\mu_s^{>}$ and $\mu_s^{<}$ throughout the structure (even at the interface).[21]

By placing these solutions into Eq. (4), the current density for $z>0$ is thus

$$j_s^{>}(z)=\frac{\sqrt{3}}{\rho_s}\left[-\gamma_1+\frac{C_1\lambda_{-s}}{\lambda_{sf}(\lambda_s+\lambda_{-s})}\exp(-z/\lambda_{sf})+\frac{\alpha}{\lambda_s}\exp(-z/\lambda_s)\right], \tag{9}$$

$$j_s^{<}(z)=\frac{\sqrt{3}}{\rho_s}\left[-\gamma_1+\frac{C_1\lambda_{-s}}{\lambda_{sf}(\lambda_s+\lambda_{-s})}\exp(-z/\lambda_{sf})-\frac{\alpha}{\lambda_s}\exp(-z/\lambda_s)\right], \tag{10}$$

$$j_{-s}^{>}(z)=\frac{\sqrt{3}}{\rho_{-s}}\left[-\gamma_1-\frac{C_1\lambda_{s}}{\lambda_{sf}(\lambda_s+\lambda_{-s})}\exp(-z/\lambda_{sf})+\frac{\beta}{\lambda_{-s}}\exp(-z/\lambda_{-s})\right], \tag{11}$$

$$j_{-s}^{<}(z)=\frac{\sqrt{3}}{\rho_{-s}}\left[-\gamma_1-\frac{C_1\lambda_{s}}{\lambda_{sf}(\lambda_s+\lambda_{-s})}\exp(-z/\lambda_{sf})-\frac{\beta}{\lambda_{-s}}\exp(-z/\lambda_{-s})\right]. \tag{12}$$

Similarly, the current density for $z<0$ can also be written down.

The above solutions contain a number of constants of the integrations which have to be determined by the boundary conditions. We assume that the electrons are subject to an average spin-dependent reflection and transmission across the interface. The detailed balancing conditions will link the current and chemical potentials at the two side of the interface. We now list these boundary conditions.

First the total current density

$$j=j_s(z)+j_{-s}(z)=j_s^{>}+j_s^{<}+j_{-s}^{>}+j_{-s}^{<} \tag{13}$$

is conserved. One can verify it immediately from Eqs. (9)–(12) that indeed

$$\frac{\partial j(z)}{\partial z}=0. \tag{14}$$

Examining the solutions for $z>0$ and $z<0$, one obtains $\gamma_1=\gamma_1'$.

Next we write down the outer-boundary condition at $z=-L$ and $z=L$ when the layer thickness L is much larger than any transport length. Then the exponential terms in Eqs. (5)–(8) can be discarded, and one has

$$\gamma_0+\gamma_1 L=V(L)=0 \tag{15}$$

and

$$\gamma_0'-\gamma_1' L=V(-L)=V_{ext}, \tag{16}$$

where we place the voltages at $x=L$ to be zero and at $x=-L$ to be the external voltage V_{ext}.

The key boundary conditions are those at the interface. We assume that the interface scattering can be characterized by the average spin-dependent transmission and reflection coefficients, but that there is no spin-flip process; then the detailed balance conditions of the spin flux across the interface are

$$j_s^{>}(0^+)=T_s j_s^{>}(0^-)-R_s j_s^{<}(0^+) \tag{17}$$

and

$$j_s^{<}(0^-)=T_s j_s^{<}(0^+)-R_s j_s^{>}(0^-), \tag{18}$$

where $T_{s(-s)}$ is the average transmission coefficient for electrons across the interface. The last set of the boundary conditions involve discontinuity of the chemical potentials at the interface. In the same spirit of the contact (Sharvin) resistance, by counting the number of electrons at two sides of the interface, one has

$$\mu_s^{>}(0^+)-\mu_s^{<}(0^+)=\mu_s^{>}(0^-)-\mu_s^{<}(0^-), \tag{19}$$

and by counting the number of electrons passing through the interface one obtains

$$T_s\mu_s^{>}(0^-)-T_s\mu_s^{<}(0^+)=AR_c j_s(0), \tag{20}$$

where $R_c=h/e^2N$ is the contact resistance, $N=A/a_0^2$ is the number of the channels, A is the cross-section area, and a_0 is the lattice constant.

Equations (15)–(20) completely determine the constants of the integration entering the chemical potentials [Eqs. (5)–(8)] and the local current density [Eqs. (9)–(12)]. It is straightforward to carry out the algebra and we are able to find all constants. For example,

$$C_1=-\frac{\sqrt{3}j\rho_s\lambda_s}{6(\lambda_s+\lambda_{-s})}\times\left\{C_0\left(\frac{\lambda_s}{T_s}-\frac{\lambda_{-s}}{T_{-s}}\right)+\left(1+\frac{\sqrt{3}}{2}\right)\times\left(\frac{R_s\lambda_s}{T_s}-\frac{R_{-s}\lambda_{-s}}{T_{-s}}\right)+\frac{\lambda_{sf}(\lambda_s+\lambda_{-s})(\lambda_s-\lambda_s')}{2\lambda_s\lambda_{-s}}\right\}, \tag{21}$$

where $C_0=\sqrt{3}R_cA/\rho_s\lambda_s$. The other constants have similar tedious expressions that we do not list here.

With these coefficients determined, we can calculate the resistance of the structure for the two magnetic layers aligned parallel and antiparallel, thereby the magnetoresistance. For the parallel alignment of the magnetization, we assume that the left and right layers are identical (but the interface reflection coefficient is arbitrary), i.e., $\rho_s=\rho_s'$ and $\lambda_s=\lambda_s'$. After carrying out the algebra, we find the total resistance is

$$R_T^{PP}\equiv\frac{V_{ext}}{Aj}=\frac{\rho_s\lambda_s}{\sqrt{3}A(\lambda_s+\lambda_{-s})}\left\{L+\frac{C_0(\lambda_s^2T_{-s}+\lambda_{-s}^2T_s)+(1+\sqrt{3}/2)(R_sT_{-s}\lambda_s^2+R_{-s}T_s\lambda_{-s}^2)}{T_sT_{-s}(\lambda_s+\lambda_{-s})}\right\}, \tag{22}$$

For the case where the two Co layers are in an antiferromagnetic configuration (AP), we identify $\rho_s=\rho_{-s}'$ and $\lambda_s=\lambda_{-s}'$. By carrying out a similar tedious calculation, we have

$$R_T^{AP}=\frac{\rho_s\lambda_s}{\sqrt{3}A(\lambda_s+\lambda_{-s})}\times\left\{L+\frac{C_0(\lambda_{-s}T_s+\lambda_sT_{-s})+(1+\sqrt{3}/2)(R_{-s}T_s\lambda_{-s}+R_sT_{-s}\lambda_s)}{2T_sT_{-s}}+\frac{\lambda_{sf}(\lambda_s-\lambda_{-s})^2}{4\lambda_s\lambda_{-s}}\right\}. \tag{23}$$

Thus the magnetoresistance is $\Delta R=R_T^{AP}-R_T^{PP}$.

The above expressions [Eqs. (22) and (23)] explicitly show that the total resistance of the system, either for a parallel or antiparallel magnetization of the two magnetic layers, cannot be written simply as a summation of the interface and the bulk resistance, but also includes additional terms which represent the transition of the electron transport from the ballistic to diffusive regions.

IV. APPLICATIONS AND RESULTS

The main difficulty in determining the conductance of a layered system is the interface scattering parameters. While the bulk parameters, such as the resistivity and the mean free paths, can be accurately measured experimentally, the interface resistance can only be determined indirectly. Therefore, it will be extremely useful to use the interface parameter from an *ab initio* calculation rather than indirectly obtained experimental data. Our formulation makes a quantitative prediction possible, since all the parameters are either from direct experimental results (for bulk parameters) or from *ab initio* data (for interface transmission coefficients).

To directly utilize the analytical results obtained in Sec. III we need to specify the effective interface transmission coefficients T_s. For a sandwich structure such as Co/Cu/Co, there are in fact two interfaces; one is Co/Cu and the other is Cu/Co. To model these two interfaces by a single interface between two Co layers, we replace the Co/Cu/Co structure by a simplified Co/Co structure; see Fig. 1. This simplification is valid as long as the thickness of the spacer layer is thinner than the transport length scale. The effective transmission coefficient T_s of the right diagram in Fig. 1 can be constructed from the two individual transmission coefficients of the left diagram, depending on the coherence of the scattering between the two interfaces. In general, we can write[19]

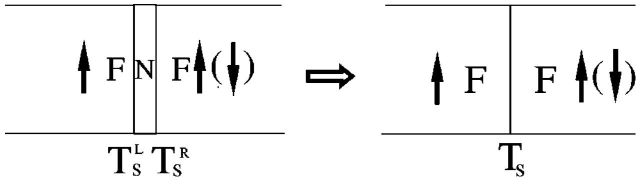

FIG. 1. The two-interface problem is modeled by an equivalent one-interface problem with an effective transmission coefficient constructed from the two transmission coefficients of the left diagram; see Eq. (24).

TABLE I. Spin-dependent transmission coefficients and magnetoresistance for a number of trilayers. α is the ratio of the mean free paths for spin-up and -down. The magnetoresistance ΔR is in units of 10^{-4} $\mu\Omega$ cm^2.

Materials	$T_\downarrow = T_\uparrow$ (AF)	$T_\uparrow$ (F)	$T_\downarrow$ (F)	ΔR $(\alpha=5.0)$	ΔR $(\alpha=1)$
Co/Cu/Co	0.34	0.76	0.22	1.1	0.19
Fe/Au/Fe	0.15	0.39	0.09	1.7	0.74
Fe/Ag/Fe	0.13	0.39	0.08	1.9	0.91
Ni/Cu/Ni	0.44	0.70	0.32	0.82	0.06

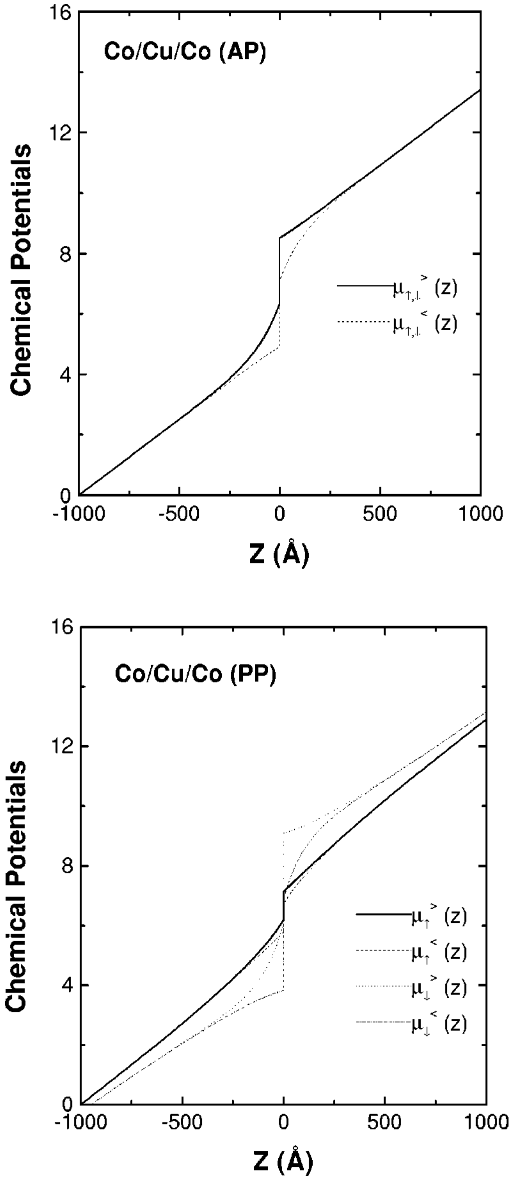

FIG. 2. The spin-dependent right-going and left-going chemical potential profiles obtained by using the transmission coefficients of Co/Cu interface derived from Stiles (Ref. 22). The impurity scattering in the layer is assumed to be spin independent with a mean free path $\lambda_s = 67$ Å, a resistivity 10 $\mu\Omega$ cm, and a spin diffusion length $\lambda_{sf} = 500$ Å. The upper and lower panels are for the magnetization of two Co layers antiparallel and parallel, respectively.

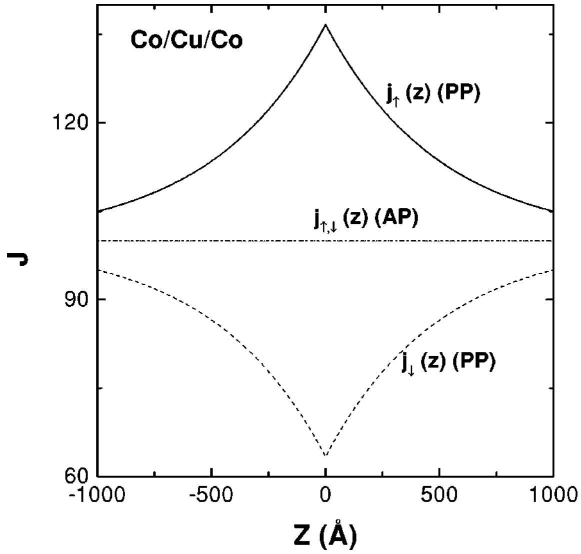

FIG. 3. The spin-dependent current density profiles by using the same parameters as those of Fig. 2.

$$T_s(\theta) = \frac{T_s^L T_s^R}{1 - 2\sqrt{R_s^L R_s^R}\cos\theta + R_s^L R_s^R}, \tag{24}$$

where T_s^L and T_s^R are the transmission coefficient across the Co/Cu and Cu/Co interfaces of the Co/Cu/Co structure, $R_s^{L(R)} = 1 - T_s^{L(R)}$ is the corresponding reflection coefficient, and θ is the phase shift of the electron wave acquired in one round trip between the two interfaces. It is rather reasonable to assume that the phase shift θ is either random due to decoherence (uncorrelated scattering) from two interfaces or almost uniformly distributed from $\theta=0$ to $\theta=2\pi$ due to large numbers of the momentum channels for the metallic system. Therefore, we may take the average over the angle in Eq. (24), and we find

$$T_s = \frac{1}{2\pi}\int_0^{2\pi} T_s(\theta)\, d\theta = \frac{T_s^L T_s^R}{1 - R_s^L R_s^R}. \tag{25}$$

Now we can utilize *ab initio* data to determine T_s. The transmission coefficients of the interfaces, e.g., Co/Cu, Fe/Au, and Ni/Cu, have been calculated by Stiles.[22] It is noted, however, that, the average transmission coefficients for the electrons going from the nonmagnetic layer to the magnetic layer are different from the electrons going from the magnetic layer to the nonmagnetic layer in Ref. 22; this is because the number of states at the Fermi levels are different for the magnetic and nonmagnetic layers. It is easy to show that the average transmission coefficient used in our detailed balance equations is simply the geometrical mean of these two coefficients, i.e., $T_s^L = \sqrt{T_s^{nm} T_s^{mn}}$ where T_s^{nm} represents the transmission coefficient from the materials n to m; those numbers are listed in Ref. 22. In Table I, we have evaluated the transmission coefficients from Eq. (25) by using the data of T_s^{nm} in Ref. 22. It is noted that when the two magnetic layers are antiparallel, $T_s^L = T_{-s}^R$, the equivalent transmission

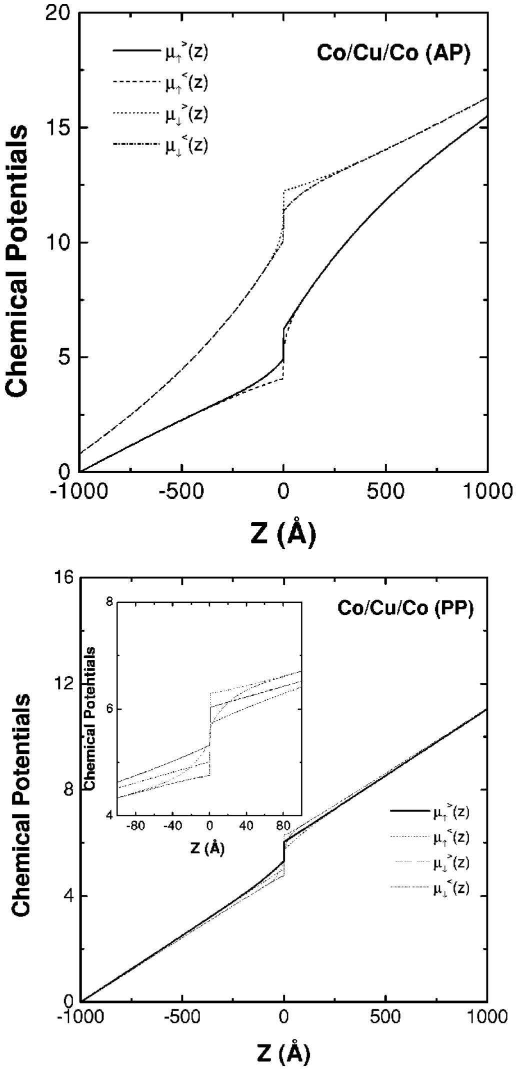

FIG. 4. The spin dependent right- and left-going chemical potential profiles in the presence of the spin-dependent bulk scattering. The transmission coefficients are derived from Ref. 22, and the bulk spin dependence of the mean free paths $\lambda_\uparrow/\lambda_\downarrow=5$.

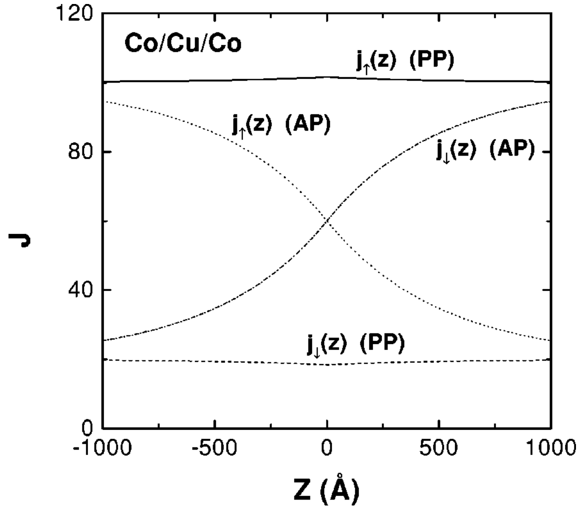

FIG. 5. The spin-dependent current density profiles in the presence of the spin-dependent bulk scattering. The parameters are same as those of Fig. 4.

coefficients calculated from Eq. (25) for spin-up and -down are identical, i.e., $T_\uparrow(AF)=T_\downarrow(AF)=T_s^L T_{-s}^L/(1-R_s^L R_{-s}^L)$.

With these specified transmission coefficients, we can quantitatively determine the effects of the interface scattering. In Fig. 2, we show the chemical potentials near the interface for the case that the bulk diffusive scattering is spin independent. In this case, the spin dependence of the chemical potentials comes solely from the interfacial ballistic scattering. One immediately notices two different length scales: the mean free path and the spin diffusion lengths. Within the distance of the mean free path, the separation of the right- and left-going electron chemical potentials are clearly seen both for the parallel and antiparallel aligned magnetic layers. This separation signals the ballistic nature of the interface scattering, and it closes when the electrons diffuse into the interior of the layers. Within the spin diffusion length, the chemical potentials for spin-up and -down electrons remain different for the parallel alignment of the two Co layers. For the antiparallel alignment, the spin-up and -down electrons have identical chemical potentials; this is because we have taken the bulk scattering to be spin independent (and the transmission coefficient is also independent of the spin).

In Fig. 3, we illustrate the spin dependence of the electric current density for Co/Cu/Co without the spin dependence of the bulk scattering. For the antiparallel alignment of the Co layers, the currents for spin-up and -down electrons are the same at the interface since both the effective interface transmission coefficient and bulk mean free path are spin independent. For the parallel alignment, the spin-up and -down electrons separates most at the interface. Since the current density in Fig. 3 included left- and right-going electrons, the spin current decays at the spin-diffusion length, i.e., the length scale of the mean free path has been integrated in calculating the current density.

Figure 4 shows the chemical potentials in the presence of the bulk spin-dependent scattering. In this case, both interface and bulk scatterings contribute to the chemical potential splitting between spin-up and -down channels. However, the different chemical potentials for the left- and right-going electrons are solely due to the interface scattering. In Fig. 5, we also illustrate the current density patterns in the presence of the bulk spin-dependent scattering. Finally, the magnetoresistance are shown in the last two columns of Table I.

V. CONCLUSIONS

We have formulated macroscopic equations which can be used to take into account both impurity scattering and interface specular reflection for current perpendicular to the plane of the layers (CPP). This approach makes the realistic estimation of the resistance and magnetoresistance possible, since full *ab initio* data can be incorporated into our calculations. Comparing to previous works on the CPP transport theories, our theory is physically more transparent in describing electron transport from ballistic to diffusive scattering. Most importantly, we have introduced different chemical potentials for right- and left-going electrons when the scattering is ballistic; this is one of the main reasons that the series resistance model for the interface scattering and bulk scattering is no more valid.

Our calculations can also serve as a criterion in determining whether the magnetoresistive head based on the traditional spin-valves has required signals when the current flows perpendicular to the layers. As the magnetoresistance in magnetic multilayers is larger for CPP than for CIP, one wishes to develop CPP-GMR heads for perpendicular magnetic recording. The present calculation shows that the optimal signals for the traditional spin valves, e.g., Co/Cu/Co, is about $\Delta R = 1.1\Omega$ for a cross section of $0.01\,(\mu\,\mathrm{m})^2$. Whether the signal of this magnitude is enough for the MR head application will be judged by signal engineers.

ACKNOWLEDGMENT

This research was supported by NSF (DMR-0076171) and National Storage Industry Consortium.

APPENDIX: DERIVATION OF MACROSCOPIC EQUATIONS

In this appendix, we derive the macroscopic equations given in Eqs. (1)–(4). We start with the semiclassical Boltzmann equation in the relaxation-time approximation,

$$v_z \frac{\partial f_{k,s}}{\partial z} - \mathrm{e}E v_z \frac{\partial f^\circ}{\partial \epsilon} = -\left[\frac{f_{k,s}-\overline{f_s}}{\tau_{ms}} + \frac{f_{k,s}-\overline{f_{-s}}}{\tau_{sf}}\right], \qquad (\mathrm{A1})$$

where $v_z = \partial\epsilon_k/\partial k_z = v_F \cos\theta$, v_F is the Fermi velocity, and θ is the angle between the direction of the velocity and the z axis, and $E = -\partial V(z)/\partial z$ is the local electric field. Two relaxation times τ_{ms} and τ_{sf} are introduced to represent the momentum and spin-flip scattering relaxation times. The overbar over $\overline{f_s}$ is the average of $f_{k,s}$ over the solid angle in the momentum space, $\overline{f_s} = (1/4\pi)\int d\Omega_{\mathbf{k}} f_{k,s}(z)$. To determine the Boltzmann distribution from Eq. (A1), we need to specify the boundary condition. In our problem, the distribution functions is $f_{k,s} = f^0 + eEv_z\tau_s\delta(\epsilon_k - \epsilon_F)$ at zero temperature for $z = \pm\infty$, where f^0 is the equilibrium distribution function. At $z=0$ the two sides of the distributions are connected via the detailed balancing conditions which are explicitly dealt with in Sec. IV. If one demands that the detailed balancing conditions be valid for *every* mode of momenta, one would have no choice except to solve Eq. (A1) numerically. In general, it is extremely difficult to solve Eq. (A1) even for a simple form of the reflection coefficients such as in the free-electron model.[7] However, in most cases, *ab initio* calculations yield average reflection and transmission coefficients across the interface.[22] Thus one may focus on the detailed balancing condition on the average of the incoming and outgoing distribution functions; this treatment is similar to the mean-field theory where the angular dependence of the scattering matrix has been omitted. Below we develop an approximate solution which will be simple and yet accurate enough to capture the average transport process across the interface.

With the picture we have discussed in Sec. II, we introduce two different chemical potentials for electrons going toward and leaving from the interface. We take the distribution function $f_{k,s}$ in the form

$$f_{k,s} = f^0 + \left(-\frac{\partial f^0}{\partial \epsilon}\right)[\mu_s^{>}\theta(k_z) + \mu_s^{<}\theta(-k_z) - g_s(k,z)], \qquad (\mathrm{A2})$$

where $\theta(x)$ is the step function. As we have emphasized that the distinction of the left- and right- going quasichemical potentials $\mu_s^{>}$ and $\mu_s^{<}$ are necessary to characterize the ballistic scattering at the interface. It is noted that the function $g_s(k_z,z)$ depends on both the magnitude and direction of the wave vector k_z.

By placing Eq. (A2) into Eq. (A1), the Boltzmann equation reads,

$$\begin{aligned} v_z\left[eE + \frac{\partial\mu_s^{>}}{\partial z}\theta(k_z) + \frac{\partial\mu_s^{<}}{\partial z}\theta(-k_z)\right] &= \frac{g_s(k_z,z)}{\tau_s} + v_z\frac{\partial g_s(k_z,z)}{\partial z} - \frac{\mu_s^{>}\theta(k_z) + \mu_s^{<}\theta(-k_z)}{\tau_s} \\ &\quad + \frac{\mu_s^{>} + \mu_s^{<} - 2\overline{g_s}}{2\tau_{ms}} - \frac{\mu_{-s}^{>} + \mu_{-s}^{<} - 2\overline{g_{-s}}}{2\tau_{sf}}, \end{aligned} \qquad (\mathrm{A3})$$

where we have defined $\tau_s^{-1} = \tau_{ms}^{-1} + \tau_{sf}^{-1}$. The above equation involves two functions, the position-dependent function of the chemical potential and the nonequilibrium distribution function $g_s(k_z,z)$ which controls the local current density. We observe that only the first term on the right-side side of Eq. (A1) exists for a homogeneous system. The remaining terms are due to spatial inhomogeneity, and fluctuate around the homogeneous result. Within the spirit of the mean-field approximation, a good trial solution is thus to assume that $g_s(k_z,z)$ has the form

$$g_s(k_z,z) = v_z\tau_s\left[eE + \frac{\partial\mu_s^{>}}{\partial z}\theta(k_z) + \frac{\partial\mu_s^{<}}{\partial z}\theta(-k_z)\right], \qquad (\mathrm{A4})$$

so that

$$\overline{g_s} = \frac{v_F\tau_s}{4}\left(\frac{\partial\mu_s^{>}}{\partial z} - \frac{\partial\mu_s^{<}}{\partial z}\right), \qquad (\mathrm{A5})$$

To examine such a tentative solution indeed being a good approximation, we place it into Eq. (A3); we obtain

$$\begin{aligned} v_z^2\tau_s^2\left[\frac{\partial^2\mu_s^{>}}{\partial z^2}\theta(k_z) + \frac{\partial^2\mu_s^{<}}{\partial z^2}\theta(-k_z)\right] &= \mu_s^{>}\theta(k_z) + \mu_s^{<}\theta(-k_z) \\ &\quad - \frac{\tau_s}{\tau_{ms}}\left[\frac{\mu_s^{>} + \mu_s^{<}}{2} - \frac{v_F\tau_s}{4}\left(\frac{\partial\mu_s^{>}}{\partial z} - \frac{\partial\mu_s^{<}}{\partial z}\right)\right] \\ &\quad - \frac{\tau_s}{\tau_{sf}}\left[\frac{\mu_{-s}^{>} + \mu_{-s}^{<}}{2} - \frac{v_F\tau_{-s}}{4}\left(\frac{\partial\mu_{-s}^{>}}{\partial z} - \frac{\partial\mu_{-s}^{<}}{\partial z}\right)\right]. \end{aligned} \qquad (\mathrm{A6})$$

Clearly, Eq. (A6) cannot be satisfied for every velocity v_z unless the chemical potentials $\mu_s^>$ or $\mu_s^<$ depend on the momentum. In fact, it is strictly true that the local potential near the interface depends on the direction of the electron momentum due to the momentum dependence of the transmission coefficient. However, as we have emphasized, we are only interested in the average over the incoming and outgoing distribution functions. Thus an average over the incoming and outgoing momenta should be taken in Eq. (A6). By replacing v_z^2 by $v_F^2/3$, we find that the above equation can be written separately for $k_z>0$ and $k_z<0$, i.e.,

$$\frac{v_F^2\tau_s^2}{3}\frac{\partial^2\mu_s^>}{\partial z^2}=\mu_s^> - \frac{\tau_s}{\tau_{ms}}\left[\frac{\mu_s^>+\mu_s^<}{2}-\frac{v_F\tau_s}{4}\left(\frac{\partial\mu_s^>}{\partial z}-\frac{\partial\mu_s^<}{\partial z}\right)\right] - \frac{\tau_s}{\tau_{sf}}\left[\frac{\mu_{-s}^>+\mu_{-s}^<}{2}-\frac{v_F\tau_{-s}}{4}\left(\frac{\partial\mu_{-s}^>}{\partial z}-\frac{\partial\mu_{-s}^<}{\partial z}\right)\right] \tag{A7}$$

and

$$\frac{v_F^2\tau_s^2}{3}\frac{\partial^2\mu_s^<}{\partial z^2}=\mu_s^< - \frac{\tau_s}{\tau_{ms}}\left[\frac{\mu_s^>+\mu_s^<}{2}-\frac{v_F\tau_s}{4}\left(\frac{\partial\mu_s^<}{\partial z}-\frac{\partial\mu_s^>}{\partial z}\right)\right] - \frac{\tau_s}{\tau_{sf}}\left[\frac{\mu_{-s}^>+\mu_{-s}^<}{2}-\frac{v_F\tau_{-s}}{4}\left(\frac{\partial\mu_{-s}^<}{\partial z}-\frac{\partial\mu_{-s}^>}{\partial z}\right)\right]. \tag{A8}$$

These two equations, along with the other two obtained by exchange s to $-s$, determine the four chemical potentials $\mu_\uparrow^>$, $\mu_\uparrow^<$, $\mu_\downarrow^>$, and $\mu_\downarrow^<$. Equations (1)–(3) are the result of taking the linear combinations of the above equations; we have defined the mean free path $\lambda_s=v_F\tau_s/\sqrt{3}$, and the diffusion length $\lambda_{sf}=[\tau_\uparrow\tau_\downarrow v_F\tau_{sf}/(3\tau_\uparrow+3\tau_\downarrow)]^{1/2}$, and we neglect the difference between τ_s and τ_{ms}. The current density is $j_s(z)=e\int v_z f_{\mathbf{k},z}d^3\mathbf{k}$. By using Eqs. (A2) and (A3), we obtain Eq. (4) for the current density.

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[1] R. Landauer, IBM J. Res. Dev. **1**, 233 (1957); in *Localization, Interaction, and Transport Phenomena*, edited by G. Bergmann and Y. Bruynseraede (Springer-Verlag, New York, 1985), p. 38; IBM J. Res. Dev. **32**, 306 (1988).
[2] Yu. V. Sharvin, Sov. Phys. JETP **48**, 984 (1965).
[3] Y. Imry and R. Landauer, Rev. Mod. Phys. **71**, S306 (1999).
[4] P.W. Anderson, D.J. Thouless, E. Abrahams, and D.S. Fisher, Phys. Rev. B **22**, 3519 (1980); P.W. Anderson, *ibid.* **23**, 4828 (1981); D.S. Fisher, and P.A. Lee, *ibid.* **23**, 6851 (1981).
[5] K.M. Schep, P.J. Kelly and G.E.W. Bauer, Phys. Rev. Lett. **74**, 586 (1995).
[6] B. Laikhtman and S. Luryi, Phys. Rev. B **49**, 17 177 (1994); C. Kunze, *ibid.* **51**, 14 085 (1995).
[7] S. Zhang and P.M. Levy, Phys. Rev. B **57**, 5336 (1998).
[8] D.R. Penn and M.D. Stiles, Phys. Rev. B **59**, 13 338 (1999).
[9] E.Y. Tsymbal and D.G. Pettifor, Phys. Rev. B **61**, 506 (2000).
[10] W.H. Butler, X.G. Zhang, and J.M. MacLaren, J. Appl. Phys. **87**, 5173 (2000).
[11] A. Shpiro and P.M. Levy, Phys. Rev. B **63**, 014419 (2001).
[12] P.M. Levy, in *Solid State Physics*, edited by H. Ehrenreich and D. Turbull (Academic, Boston, 1994), Vol. 47, p. 367.
[13] E.Y. Tsymbal and D.G. Pettifor, in *Solid State Physics,* edited by H. Ehrenreich and D. Turbull (Academic, Boston, 2000), Vol. 56, p. 113.
[14] V.K. Dugaev, V.I. Litvinov, and P.P. Petro, Phys. Rev. B **52**, 5306 (1995).
[15] C.S. Chu and R.S. Sorbello, Phys. Rev. B **38**, 7260 (1988); R.S. Sorbello, *ibid.* **39**, 4984 (1989).
[16] M.Ye. Zhuravlev, H.O. Lutz, and A.V. Vedyayev, Phys. Rev. B **63**, 174409 (2001).
[17] L.R. Tagirov, B.P. Vodopyanov, and K.B. Efetov, Phys. Rev. B **63**, 104428 (2001).
[18] H.E. Camblong, Phys. Rev. B **51**, 1855 (1995).
[19] S. Datta, in *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).
[20] P.C. van Son, H. van Kempen, and P. Wyder, Phys. Rev. Lett. **58**, 2271 (1987); M. Johnson and R.H Silsbee, Phys. Rev. B **37**, 5312 (1988).
[21] T. Valet and A. Fert, Phys. Rev. B **48**, 7099 (1993).
[22] M.D. Stiles, J. Appl. Phys. **79**, 5805 (1996).