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Theory of parallel and perpendicular transport in magnetic multilayers with interdiffusion-induced correlation at interfaces

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Abstract. On the basis of the tight-binding approximation and by including the correlation of interdiffusion impurities at interfaces, a quantum transport theory is developed for both the current in the plane (CIP) and the current perpendicular to the plane (CPP) of the layers in magnetic multilayers. It is found that the CIP and CPP transport properties are quite different, the CPP transport exhibiting self-averaging behaviour. We show that the interdiffusion-induced correlation at interfaces can enhance the giant magnetoresistance in both the CIP and CPP geometries.

1. Introduction

The giant magnetoresistance (GMR) in magnetic multilayers such as $(\text{Fe/Cr})_n\text{Fe}$ and $(\text{Co/Cu})_n\text{Co}$ has attracted much recent attention as regards the currents both in the plane of the layers (CIP) [1, 2] and perpendicular to the plane of the layers (CPP) [3, 4]. It is widely accepted that the GMR effect results from the different scattering rates for spin-up and spin-down electrons. For CIP geometry, the spin-dependent conduction properties are averaged over the lengths of the electron mean free path for spin up and spin down separately. For CPP geometry, an additional spin-accumulation effect leads to a nonuniform electric field, the effect of which needs to be considered.

A quasiclassical method based on the Boltzmann equation [5–7] and a quantum approach starting from the Kubo formula [8, 9] as well as the Landauer–Büttiker formalism [10] have been developed to address the GMR in magnetic multilayers. The relative contributions to the scattering rate from bulk and interfacial scattering processes are considered to be important [11]. Although there is some controversy about whether the spin-dependent scattering is primarily interfacial or bulk scattering, it has been proposed that both the strength and the spin dependence of the scattering at interfaces between layers are stronger than those in the bulk of the layers, and so the scattering at the interfaces plays a crucial role in producing the GMR effect [12]. It is not surprising that the scattering is stronger at interfaces, as the concentration of impurities is usually higher at interfaces. In an attempt to understand the stronger spin dependence of scattering at interfaces, Zhang and Levy [13] pointed out recently that the scattering between randomly distributed impurities in the bulk is phase incoherent, while that of a pair of interdiffusion impurities at the interface is phase coherent. A single-cluster coherent potential approximation (CPA) method has been applied

to the correlated interdiffusion impurities at interfaces [13, 14]. The physical content of the correlation is as follows: for an interdiffusion interface composed of several monolayers (MLs), the occupation state of a site in one of the MLs is related to that of the adjacent site in the neighbouring ML. For instance, for an interface composed of ML1 (mainly composed of A atoms) and ML2 (mainly composed of B atoms), in the dilute-concentration limit, if a site in ML2 is occupied by an A atom interdiffused from ML1, then the adjacent site in ML1 must be occupied by a B atom interdiffused from ML2. In the weak-scattering limit, it is shown that the effect of the interdiffusion-induced correlation on the interfacial scattering is related to the off-diagonal part of the coherent potential (self-energy) and that the correlation enhances the spin-dependent scattering from the interfaces [14].

Since the calculation of the correlated interfacial scattering in reference [14] dealt only with the CIP transport in a single-interface system, it is highly desirable to apply the CPA approach to study both CIP and CPP magnetotransport in realistic magnetic multilayers and then to examine the effect of the correlated scattering on the GMR. In this paper we will make an effort to do this. First, we wish to derive analytical expressions for the CIP and CPP conductivities by using the Kubo formula under the tight-binding approximation (TBA). The interfacial scattering is determined by the self-energy, which includes off-diagonal elements, in connection with the correlation of interdiffusion impurities at interfaces. By applying the Green's function approach and the Kubo formula in real space, we obtain a microscopic quantum description of the CIP conductivity σ_x and CPP conductivity σ_z in magnetic multilayers, with the correlation at interfaces being taken into account. It is found that the CIP and CPP transport properties are quite different. The result for σ_z is close to that obtained from an effective-relaxation-time method, indicating that there is a global self-averaging effect in the CPP transport, while in the CIP geometry such an averaging effect exists only in the homogeneous limit. We examine a further correlation effect on the GMR by using the conductivity formula derived. Calculations show that the scattering from interdiffusion impurities at interfaces enhances the magnitude of the magnetoresistance.

2. The model

Consider a magnetic multilayer structure, with a great number of well-lattice-matched bilayers stacked along the z -axis. Each bilayer is composed of a ferromagnetic (A) film of L_0 monolayers and a nonmagnetic (B) film of L_1 monolayers. First, we consider an ideal structure with sharp interfaces, for which there is neither interdiffusion of atoms A and B nor geometrical roughness, as shown in figure 1(a). If reflection effects at interfaces are neglected, the single-particle retarded Green's function in the momentum representation may be given by

$$G^{0,s}(\mathbf{q}, \omega) = \frac{1}{\omega - \varepsilon_q^s + i/2\tau_0} \quad (1)$$

where ε_q^s is the single-particle energy. Since we will focus our attention on the interface effect on the GMR qualitatively, for simplicity, we assume that

$$\varepsilon_q^s = \varepsilon_0^s + 2t[\cos(q_x a) + \cos(q_y a) + \cos(q_z a)]$$

in the tight-binding band of a simple cubic lattice with a the lattice constant, in which ε_0^s is spin dependent [13, 14]. The small imaginary part comes from the weak bulk scattering and τ_0 is the average relaxation time, which has been assumed independent of spin and position. With the aid of Fourier transformation, one obtains [14]

$$G_{\alpha\beta}^{0,s}(\mathbf{q}_{\parallel}, \omega) = -i g_s e^{-i\tilde{\theta}_s |\alpha - \beta|} \quad (2)$$

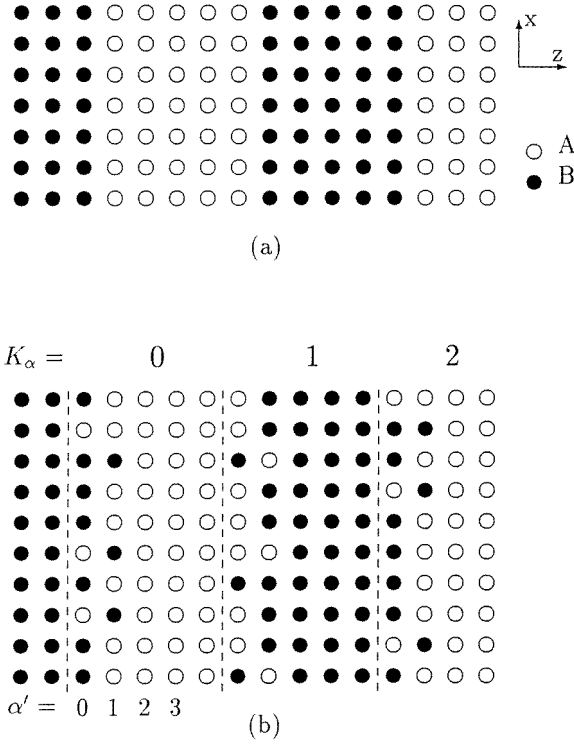


Figure 1. Profiles of multilayer structures with sharp interfaces (a) and with double-monolayer interdiffusional interfaces (b).

where

$$\tilde{\theta}_s = \cos^{-1}(\cos \theta_s + i/4t \tau_0) \approx \theta_s - i\theta'_s$$

and

$$g_s = 1/(2t \sin \theta_s)$$

with

$$\cos \theta_s = (\omega - \varepsilon_0^s)/2t - \cos(q_x a) - \cos(q_y a) \quad \text{and} \quad \theta'_s = 1/(4t \tau_0 \sin \theta_s).$$

Owing to the diffusional or geometrical roughness, an interface between neighbouring A and B layers contains A and B atoms. Such an interface may include several monolayers; in the present paper we only consider the case in which each interface contains two monolayers [13, 14], as shown in figure 1(b). We use two integers (K_α , α') to denote the α th monolayer, corresponding to the α' th plane in the K_α th layer, where $0 \leq \alpha' \leq L_0 - 1$ for even K_α and $0 \leq \alpha' \leq L_1 - 1$ for odd K_α . For convenience, both monolayers of each interface are considered to belong to the layer on their right-hand side, i.e., $\alpha' = 0$ and 1 for the two monolayers of each interface. The translational invariance in the x - y plane, which is destroyed by impurities distributed randomly at the interfaces, can be restored by carrying out an appropriate averaging procedure, so the spin-dependent self-energy Σ of each interface is site diagonal with respect to the coordinates in the x - y plane. As a result, the plane indices (K_α , α') are sufficient to denote the matrix element of the self-energy. Its

off-diagonal elements may exist due to the correlation among impurities at each interface [14]. The self-energy can be written as

$$\Sigma_{\alpha\beta}^s = \begin{cases} iI_{\alpha'\beta'}^s & \text{when } K_\alpha = K_\beta = 4n \text{ or } 4n + 1 \text{ and } \alpha', \beta' = 0 \text{ or } 1 \\ iI_{\alpha'\beta'}^s & \text{when } K_\alpha = K_\beta = 4n + 2 \text{ or } 4n + 3 \text{ and } \alpha', \beta' = 0 \text{ or } 1 \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

Here I is the imaginary part of the self-energy, which is assumed to be very small compared with the width of the energy band. The real part of the self-energy has been neglected, since it can be absorbed as a redefinition of the energy reference level. $s = \uparrow$ and \downarrow denote the magnetization directions; $s' = s$ for a ferromagnetic configuration and $s' = -s$ for an antiferromagnetic configuration. $K_\alpha = \text{even (odd)}$ stands for the ferromagnetic (nonmagnetic) layers.

In the presence of impurity scattering at interfaces, the single-particle Green's function can be obtained from the Dyson equation

$$G_{\alpha\beta}^s = G_{\alpha\beta}^{0,s} + \sum_{\gamma,\delta} G_{\alpha\gamma}^{0,s} \Sigma_{\gamma\delta}^s G_{\delta\beta}^s \quad (4)$$

where, for brevity, the common arguments $\mathbf{q}_\parallel = (q_x, q_y)$ and ω have been omitted.

For the CIP conduction, there is no spin-accumulation effect and the electric field is uniform everywhere; so, from the Kubo formula, the average conductivity in the x - y plane for spin s may be written as

$$\sigma_x^s = \lim_{N \rightarrow \infty} \frac{1}{2Na} \sum_{\alpha,\beta=-N}^N \frac{e^2}{4\pi^3} \int' d^2q_\parallel v_x^2 |\text{Im } G_{\alpha\beta}^s(\mathbf{q}_\parallel, E_F)|^2 = \frac{e^2}{4\pi^3 a} \int' d^2q_\parallel v_x^2 Q_s(\mathbf{q}_\parallel) \quad (5)$$

where $v_x = \partial \varepsilon_q / \partial q_x$ is the velocity along the x -axis, $2N$ is the total number of monolayers of the multilayer structure and

$$Q_s = \lim_{N \rightarrow \infty} (1/2N) \sum_{\alpha,\beta=-N}^N |\text{Im } G_{\alpha\beta}^s|^2.$$

The primes on the integral signs indicate that the limit of the integration is [14]

$$-1 \leq (E_F - \varepsilon_0^s)/2t - \cos(q_x a) - \cos(q_y a) \leq 1.$$

3. The method

3.1. Weak interfacial scattering

To the first-order approximation of the self-energy, equation (4) yields

$$G_{\alpha\beta}^s = G_{\alpha\beta}^{0,s} + G_{\alpha\beta}^{(1),s} \quad \text{with } G_{\alpha\beta}^{(1),s} = \sum_{\gamma\delta} G_{\alpha\gamma}^{0,s} \Sigma_{\gamma\delta}^s G_{\delta\beta}^{0,s}.$$

It follows from equation (3) that the summations over γ and δ can be divided into three parts: $\gamma, \delta < \alpha$; $\alpha \leq \gamma, \delta \leq \beta$; and $\gamma, \delta > \beta$ (without loss of generality, we have assumed that $\alpha < \beta$). In the case of weak interfacial scattering, the dominant contribution to the sum of the terms $|\text{Im } G_{\alpha\beta}^s|^2$ is found from those terms with $\alpha \leq \gamma, \delta \leq \beta$, as they are proportional to $\exp(-i\tilde{\theta}_s|\beta - \alpha|)$, while the other terms are proportional to $\exp(-i\tilde{\theta}_s|\beta + \alpha - \gamma - \delta|)$. As a result, we make the approximation of retaining only the terms with $\alpha \leq \gamma, \delta \leq \beta$. Physically, such an approximation implies that, in the calculation of the transmission

amplitude of the particles, we neglect the interfacial reflection and retain only those terms that relate to a particle transmitting directly from site α to site β . This is reasonable when the interfacial scattering is not strong (small I), as has been assumed before [15]. Then, we obtain

$$G_{\alpha\beta}^{(1),s} \approx -ig_s^2 e^{-i\tilde{\theta}_s|\beta-\alpha|} \sum_i V_i \quad (6)$$

where the summation is over all interfaces between sites α and β , and

$$V_i = I_{00}^i + I_{11}^i + \cos\theta_s(I_{01}^i + I_{10}^i)$$

can be regarded as an effective self-energy of the i th interface.

Substituting $G_{\alpha\beta}^s$ given by equations (2) and (6) into equation (5), in the weak-bulk-scattering limit ($\theta'_s \ll 1$), we obtain [14]

$$Q_s \approx g_s \tau_0 (1 - \eta_s + O(\eta_s^2)) \quad (7)$$

where $\eta_s = -2(V_s + V_{s'})\tau_0/L$ ($\eta_s > 0$) represents the strength of the interfacial scattering relative to that of the bulk scattering, with $L = L_0 + L_1$ being the thickness of one period of the multilayer.

3.2. The self-averaging method

Equation (7) is only suitable for use in the case where $\eta_s \ll 1$. It requires that the effect of the interfacial scattering is much smaller than that of the bulk scattering. In most magnetic multilayers, however, the interfacial scattering may dominate over their transport properties. To obtain a more reasonable expression, in this subsection, we apply a self-averaging method, in which the effect of interfacial scattering is averaged and is equivalent to an effective bulk scattering. On using an effective bulk relaxation time τ_e^s including the interfacial scattering effect, equation (7) is replaced by $Q_s = g_s \tau_e^s$. For small η_s , we have

$$\tau_e^s(V) = \tau_0(1 + 2V\tau_0/L) \quad (8)$$

where $V = V_s + V_{s'}$. If we consider V to be equal to V_0 plus a small increment δV , and $\tau_e^s(V_0)$ as the effective bulk relaxation time of the self-energy V_0 , equation (8) will be modified into

$$\tau_e^s(V_0 + \delta V) = \tau_e^s(V_0)(1 + 2\delta V \tau_e^s(V_0)/L)$$

where $\delta V \ll L/\tau_0$. It then follows that τ_e^s satisfies the differential equation

$$\frac{d\tau_e^s}{dV} = \frac{2\tau_e^{s2}}{L} \quad (9)$$

with the initial condition $\tau_e^s(0) = \tau_0$. The solution of equation (9) is

$$\tau_e^s = \frac{\tau_0}{1 + \eta_s}. \quad (10)$$

Correspondingly, from equation (5) the conductivity is obtained as

$$\sigma_x^s = \frac{e^2}{4\pi^3 a} \int' d^2 q_{\parallel} v_x^2 g_s \frac{\tau_0}{1 + \eta_s}. \quad (11)$$

Equation (11) is a result obtained under the self-averaging approximation, in which the effect of interfacial scattering is included in an effective bulk scattering. This result is valid in two cases. One is the homogeneous limit, regardless of whether the interfacial scattering is weak or strong. Another is that in which the interfacial scattering is weak compared with the bulk scattering, with the result that η_s is quite small.

3.3. Relatively strong interfacial scattering

Even in the case of weak interfacial scattering, for which the strength of the interfacial scattering is relatively strong compared with the bulk scattering ($\eta_s > 1$), the above perturbation calculations may not be applicable. In what follows, we start directly from the Dyson equation, expression (4), and calculate the Green's function. Since the interfacial scattering is assumed to be small, we can still neglect the interfacial reflection as we did in subsection 3.1; thus the amplitude of particles passing through an interface would only decay by a certain factor, each interface contributing a transmission factor \tilde{t} . Thus, the Green's function can be written as

$$G_{\alpha\beta}^s = -ig_s e^{-i\tilde{\theta}_s(\beta-\alpha)} \prod_i \tilde{t}_i \quad (12)$$

where \tilde{t}_i is the transmission amplitude of the i th interface between site α and β . For $\alpha = (K_i, \alpha')$ with $\alpha' = 0$ or 1 and $\beta = (K_i, \beta')$ with $\beta' > \alpha'$, substitution of

$$G_{\alpha'\beta'}^s = \tilde{t}_{i,\alpha'} G_{\alpha'\beta'}^0$$

into the Dyson equation yields

$$\tilde{t}_{i,\alpha'} = 1 - g_s \sum_{\gamma,\delta=0}^1 e^{-i\theta_s(\alpha'-\delta+|\gamma-\alpha'|)} I_{\gamma\delta}^i \tilde{t}_{i,\delta} \quad (13)$$

where $\tilde{t}_{i,\alpha'}$ is the transmission factor of the i th interface when a particle transmits from site $\alpha' = 0, 1$ to site β' . From equation (13), we have

$$\tilde{t}_{i,0}^{-1} = [1 - g_s(I_{00}^i + e^{-i\theta_s} I_{10}^i)][1 - g_s(I_{11}^i + e^{i\theta_s} I_{01}^i)] - g_s^2 e^{2i\theta_s} (I_{00}^i + e^{i\theta_s} I_{10}^i)(I_{11}^i + e^{i\theta_s} I_{01}^i) \quad (14)$$

where the second term represents the repeated reflections between the two monolayers of the i th interface. This term is small relative to the first term, and so can be neglected. When a particle at $\alpha' = 0$ transfers to site β' , it passes through both monolayers of the interface. Since \tilde{t}_i is the transmission factor contributed by this interface, we have $\tilde{t}_i = \tilde{t}_{i,0}$, and thus

$$\tilde{t}_i^{-1} \approx [1 - g_s(I_{00}^i + e^{-i\theta_s} I_{10}^i)][1 - g_s(I_{11}^i + e^{i\theta_s} I_{01}^i)]. \quad (15)$$

It is easily seen from equation (15) that \tilde{t}_i^{-1} for a double-monolayer interface can be regarded as a product of two terms, each corresponding to the contribution of one of the two monolayers. Their effective self-energies are $\Sigma_{00} + e^{-i\theta_s} \Sigma_{10}$ and $\Sigma_{11} + e^{i\theta_s} \Sigma_{01}$.

4. CIP and CPP conductivities

Equation (15) shows that both the diagonal and off-diagonal parts of the self-energy contribute to the interfacial scattering. From equations (5) and (12), we can find the CIP conductivity for each spin channel. The total CIP conductivity $\sigma_x = \sum_s \sigma_x^s$ is obtained as

$$\sigma_x = \frac{e^2}{4\pi^3} \sum_s \int' d^2 q_{\parallel} v_x^2 \frac{\tau_0}{2t \sin \theta_s} \left[1 - \frac{2\tau_0 t \sin \theta_s}{L} U_{ss'} \right] \quad (16)$$

with

$$U_{ss'} = \frac{(1 - T_s)[(1 + T_s e^{-2\theta'_s L_0})(1 - e^{-2\theta'_s L_1}) + (1 + T_s e^{-2\theta'_s L_1})(1 - e^{-2\theta'_s L_0}) \Delta_{ss'}]}{1 - T_s T_{s'} e^{-2\theta'_s L}}$$

where $T_s = \tilde{t}_s^2$ is the momentum- and spin-dependent interfacial transmission coefficient, and

$$\Delta_{ss'} = (1 + T_s^2 e^{-2\theta'_s L}) / (1 + T_s T_{s'} e^{-2\theta'_s L}).$$

It is interesting to notice that equation (16) has a form similar to the result obtained from the semiclassical approach based on the Boltzmann equation [7], indicating a close connection between the present quantum method and the semiclassical approach. The difference between these two approaches is that in the semiclassical approach the interfacial transmission coefficients are phenomenological parameters independent of the momentum, while they are momentum dependent in the present work, and are determined by the self-energy of the interfacial scattering. Also, the density of states (DOS) in the integral of equation (16) is of tight-binding type, while the DOS is usually free-electron-like in the semiclassical approach [7].

In the homogeneous limit, the degree of decay of a particle's amplitude should be very small after the particle passes through one layer; from expression (12) for the Green's function, it follows that $T_s \rightarrow 1$ and $\theta'_s L \ll 1$. In such a case, it is easy to verify that equation (16) reduces to the result derived from the self-averaging method, equation (11), as expected. On the other hand, in the opposite limit (the local limit), where $\theta'_s L_0 \gg 1$ and $\theta'_s L_1 \gg 1$, the second term in equation (16) is very small, indicating that the interfacial scattering has little effect on the CIP conductivity.

We next calculate the CPP conductivity. Unlike in the CIP geometry where the electric field is uniform, for the CPP geometry, spin-accumulation effects must be taken into account, so the actual electric field is no longer uniform. When an electric field is applied along the z -axis, if the spin-flip process can be neglected, a general formula for the current density with spin s at site α is

$$J_\alpha^s = \int d^2 q_\parallel j_\alpha^s \quad (17)$$

with

$$j_\alpha^s = \frac{e^2}{4\pi^3} v_z^2 \sum_\beta |\text{Im} G_{\alpha\beta}^s|^2 E_\beta^s \quad (18)$$

where $v_z = \partial \varepsilon_q / \partial q_z$ is the velocity along the z -direction. Due to the translational invariance in the x - y plane and the current conservation for each spin channel, the z -direction current density J_α^s should be independent of site α . Such a condition can be satisfied as long as j_α^s is assumed to be independent of α .

We make the definition $B_\alpha = 1 + (T_i^{-1} - 1)/2(1 - e^{-2\theta'_i})$ when α belongs to the i th interface and $B_\alpha = 1$ otherwise. Multiplying B_α by both sides of equation (18) and then performing summations over α , we find

$$j^s \sum_\alpha B_\alpha = \frac{e^2}{4\pi^3} v_z^2 \frac{g_s^2}{1 - e^{-2\theta'_s}} \sum_\beta E_\beta^s \quad (19)$$

where we have used the condition that $j_\alpha^s = j^s$ is independent of α . Since the average electric field is given by

$$\bar{E} = (1/2N) \sum_{\beta=-N}^N E_\beta^s$$

then, from equations (17) and (18), the conductivity $\sigma_z^s = J^s/\bar{E}$ is readily obtained. The total CPP conductivity is thus

$$\sigma_z = \sum_s \sigma_z^s \quad \text{with } \sigma_z^s = \frac{e^2}{4\pi^3} \int' d^2q_{\parallel} v_z^2 \frac{\tau_0}{2t \sin \theta_s} \frac{1}{1 + 2\tau_0 t \sin \theta_s (T_s^{-1} + T_{s'}^{-1} - 2)/L}. \quad (20)$$

Substituting $T_s^{-1} = \tilde{t}_s^{-2} \approx (1 - 2g_s V_s)$ into equation (20), we find that the CPP conductivity has a form very similar to equation (11) derived from the effective-relaxation-time approximation, but is quite different from equation (16). Note that equation (20) is applicable not only in the homogeneous limit, but also in more general cases, indicating that the CPP transport has a self-averaging effect due to the spin accumulation. It follows from equation (20) that the CPP resistance can be regarded as a network in which the resistances of the two spin channels are in parallel; for each spin channel, the resistances of all of the bulk layers and interfaces are in series. Unlike in the CIP case, if $T \rightarrow 0$, the CPP conductivity given by equation (20) vanishes, because the electric currents along the z -axis must propagate through all of the interfaces. Only in the homogeneous limit do the CIP transport and CPP transport exhibit the same behaviour.

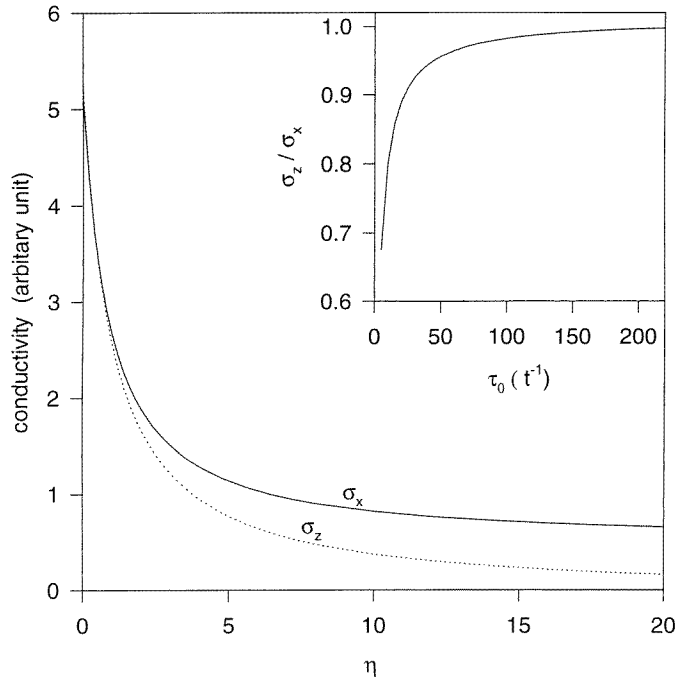


Figure 2. The conductivities σ_x and σ_z as functions of η in a nonmagnetic multilayer, with $\varepsilon_0^\uparrow = \varepsilon_0^\downarrow = 0$, $L_0 = L_1 = 10$ and $\tau_0 = 50$. The inset shows σ_z/σ_x as a function of τ_0 with a fixed $\eta = 1$.

5. Results and discussion

We now calculate numerically the CIP and CPP conductivities in a magnetic multilayer structure. Figure 2 shows σ_x and σ_z as functions of the interfacial scattering strength in a

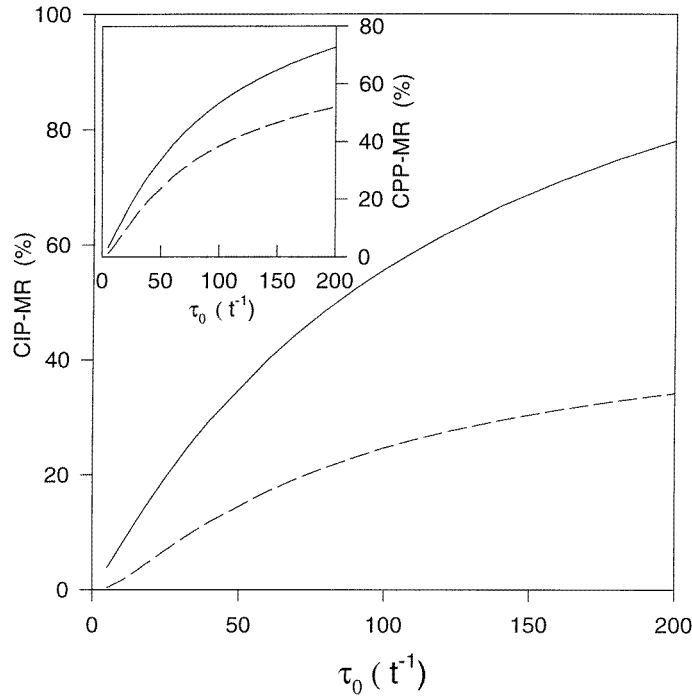


Figure 3. The CIP MR and CPP MR as functions of τ_0 . The solid line and the dashed line correspond to the completely correlated case and the uncorrelated case, respectively.

nonmagnetic multilayer structure. As the interfacial scattering is weak compared with the bulk scattering ($\eta \ll 1$), the bulk scattering dominates both the CIP and CPP transport, so σ_z is very close to σ_x . With increasing interfacial scattering, σ_z drops more quickly than σ_x . In the large- η limit, σ_z tends toward zero while σ_x tends toward a finite value. For a given interfacial scattering strength (fixed η), σ_z and σ_x are close to each other for large τ_0 , as shown in the inset of figure 2. In such a homogeneous case, the CIP transport has a self-averaging effect like the CPP transport and thus can also be described by an effective-relaxation-time method.

For magnetic multilayers, both the CIP and CPP conductivities are expressed in terms of the spin-dependent interfacial transmission coefficients, which are determined by the self-energy of the interface. It has been shown [14] that the off-diagonal part of the self-energy comes from the correlation between the impurities at the two monolayers of each interface, and that the degree of correlation can be described by a parameter ξ with $0 \leq \xi \leq 1$, where $\xi = 0$ and 1 correspond to the uncorrelated and completely correlated cases, respectively. In the weak-scattering limit, the off-diagonal elements $I_{01}^s (=I_{10}^s)$ and the diagonal elements $I_{00}^s (=I_{11}^s)$ satisfy a simple relation [14]:

$$\frac{I_{01}^s}{I_{00}^s} = -\xi \gamma_s \quad (21)$$

where

$$\gamma_s = \left(\int' \cos \theta_s \, d^2 q_{\parallel} / \sin \theta_s \right) / \left(\int' d^2 q_{\parallel} / \sin \theta_s \right)$$

is spin dependent due to the spin-dependent limits of the integrations. In the following, this relation will be used in our calculation to examine the effect of correlation on the GMR.

Next let us calculate the MR, which is defined as $(\sigma_F - \sigma_A)/\sigma_A$, with σ_F and σ_A the conductivities in the ferromagnetic and antiferromagnetic cases, respectively. In figure 3, including its inset, we plot the CIP MR and CPP MR as functions of the bulk relaxation time τ_0 in two limiting cases where $\xi = 0$ (dashed lines) and $\xi = 1$ (solid lines), by taking $\varepsilon_0^\uparrow = E_F + 3t$, $\varepsilon_0^\downarrow = E_F - 3t$, $L_0 = 10$ and $L_1 = 5$. In the absence of correlation, the maximum interfacial transmission coefficients ($\sin\theta_s = 1$) are taken to be $T_\uparrow^0 = 0.95$ for spin up and $T_\downarrow^0 = 0.8$ for spin down. It is found that the MR always increases with τ_0 , since the weight of spin-dependent interfacial scattering increases while that of bulk scattering decreases with increasing τ_0 . On the other hand, the MR in the completely correlated case is much greater than that in the uncorrelated case, indicating that the correlation can enhance GMR.

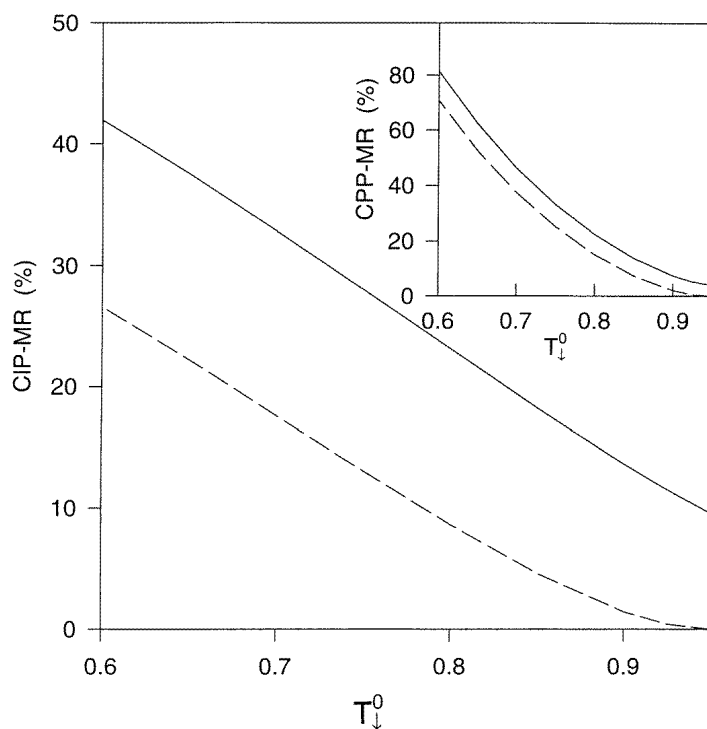


Figure 4. The CIP MR and CPP MR as functions of the interfacial transmission coefficient T_\downarrow^0 in the case of complete correlation (solid line) and no correlation (dashed line).

Figure 4, including its inset, shows the CIP MR and CPP MR as functions of the interfacial transmission coefficient T_\downarrow^0 in the two cases where $\xi = 0$ (dashed lines) and $\xi = 1$ (solid lines), with $\tau_0 = 30$, and the other parameters the same as for figure 3. As the asymmetry of the interfacial scattering decreases, the MR always decreases in both cases. It is worth noticing that, if the scattering potential at the interfaces did not depend on the spin ($T_\downarrow^0 = T_\uparrow^0$), the MR in the uncorrelated case would vanish while a nonzero MR would still exist in the correlated case. In the latter case, the interfacial scattering is related not only to the scattering potential, but also to the spin-dependent band structures. It is

easily seen from equation (21) that the ratio of the off-diagonal element to the diagonal one is related to the band structure. Thus, even if the diagonal parts of the self-energies are assumed spin independent, the off-diagonal parts may still be spin dependent because of the spin-dependent band structure in the magnetic multilayers, resulting in spin dependence of the interfacial scattering and the MR.

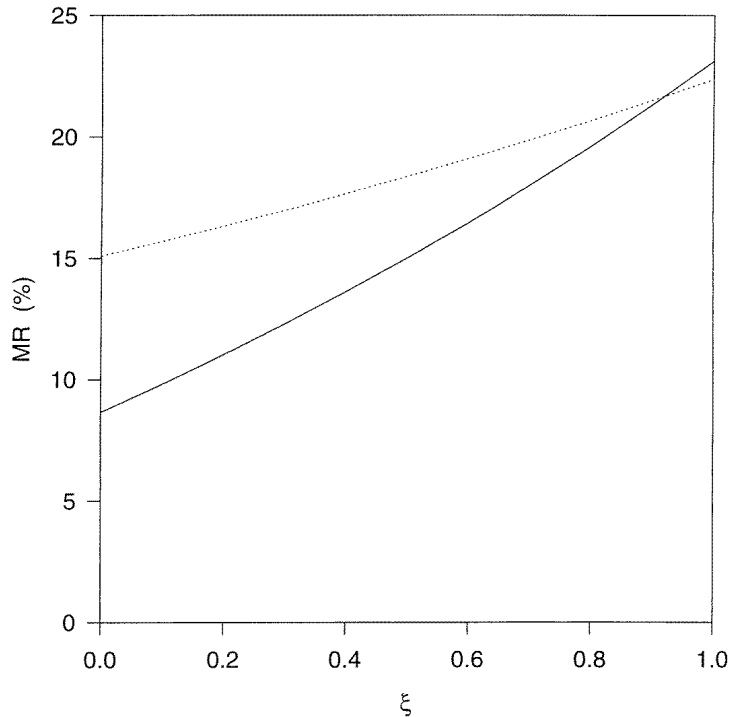


Figure 5. The CIP MR (solid line) and CPP MR (dashed line) as functions of the correlation parameter ξ , with $\tau_0 = 30$, and the other parameters the same as for figure 3.

The correlation parameter ξ was calculated in reference [14] by using a simple diffusion model. It was found that ξ increases with decreasing concentration of impurities at interfaces, and reaches its maximum ($\xi = 1$) in the dilute limit. In figure 5, we plot the CIP MR (solid line) and CPP MR (dashed line) against the correlation parameter ξ . We see that as ξ increases, the magnitude of the MR increases. In magnetic multilayers, when the interfacial roughness increases, the interfacial scattering strength increases and the correlation decreases, the two changes having opposite effects on the MR. As a result, the GMR is expected to be maximized at a particular interfacial roughness.

In summary, by including the interdiffusion-induced correlation of impurities at interfaces, we have developed a microscopic quantum description of the CIP and CPP conductivities in a magnetic multilayer under the tight-binding band approximation. Analytical formulae for σ_x and σ_z are obtained. It is found that there are global self-averaging effects for the CPP transport, while such effects exist only in the homogeneous limit in the CIP geometry. We have examined the correlation effect and found that it can enhance the value of the magnetoresistance. We conclude that the correlation at interfaces plays an important role in the GMR.

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- [15] Under this approximation, the contribution to the total transmission from the multi-reflection processes has been neglected.