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Semiclassical concepts in magnetoelectronics

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Abstract

Semiclassical theories of electron and spin transport in metallic magnetic structures are reviewed with emphasis on the role of disorder and electronic band structures in the current perpendicular to the interface plane (CPP) transport configuration. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Electron transport in layered magnetic systems can be directed parallel or perpendicular to the interfaces. The physics of transport in the latter, so-called current perpendicular to the plane (CPP) configuration, studied first by the Michigan State University Group with superconducting contacts [1,2] and by Gijs *c.s.* in microstructured pillars at arbitrary temperatures [3], has been reviewed quite recently [4,5]. The topic remains to attract the interest of the community and new insights have been obtained on issues as first-principles calculations of transport in disordered multilayers, phase coherence effects, transport with non-collinear magnetizations and spin-torques induced by applied currents. The present paper briefly reviews and compares these novel developments. Related topics of interest are superconductor–ferromagnet hybrids [6,7], spin-injection into carbon nanotubes [8,9] and semiconductors [10,11] or many-terminal devices [12].

Most studies have been carried out on multilayers consisting of many bilayer periods. In earlier studies attention was focussed on collinear magnetization profiles, i.e. that with antiparallel or parallel magnetization vectors for neighbouring layers. These experiments are well fitted by the so-called 2-channel series resistor model (2CSRM), which is discussed in the light of recent developments in Section 2. In Section 3 novel theoretical approaches are reviewed, which describe non-collinear configurations.

2. Collinear magnetization

The experiments of perpendicular transport in magnetic multilayers are well described by the 2CSRM, i.e. an equivalent electric circuit of two spin channels in parallel, in which the resistance of each channel is the sum of the bulk and interface resistances. When all magnetizations are parallel the total resistance R_T of a ferromagnetic/normal metal (F/N) multilayer of M double layers reads

$$AR_T = M\left[\rho^{(N)}d_N + \sum_s(\rho_s^{(F)}d_F + 2AR_s^{N/F})\right], \quad (1)$$

where A is the cross-section of the sample, $\rho^{(N)}$ is the resistivity of the bulk normal metal, $\rho_s^{(F)}$ is the resistivity of the ferromagnet for spin direction s, d_N and d_F are the layer thicknesses and $R_s^{N/F}$ are the spin-dependent interface resistances. The five parameters $\rho^{(N)}$, $\rho_s^{(F)}$, and $R_s^{N/F}$ can be determined accurately by fitting experiments on numerous samples with different layer thicknesses and for antiparallel as well as parallel mag-

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netic configurations [1,2]. It was soon realized that the microscopic basis was to be found in semiclassical arguments [13,14]. The most flexible theoretical framework turned out to be the linearized Boltzmann equation in the relaxation time approximation by Valet and Fert [15], which also included spin-flip processes. In this model the distribution function or local chemical potential f_s for spin s in the F or N bulk materials is governed by the one-dimensional diffusion equation

$$\frac{\partial^2 f_s(x)}{\partial x^2} = \frac{1}{2}\frac{f_s(x) - f_{-s}(x)}{l_{sf}^2}. \tag{2}$$

where σ_s is the conductivity for spin-flip processes are included in terms of the spin-diffusion length l_{sf}. Interfaces were treated as thin regions with a different (low) mobility. The current for spin s then reads

$$j_s(x) = \sigma_s \frac{\partial f_s(x)}{\partial x}, \tag{3}$$

When $l_{sf} \gg d$ the results are identical to the 2CSRM. However, this treatment is incomplete in that the discontinuities in the electronic structure at heterointerfaces are disregarded, which are essential for the electron transport properties since they scatter electrons even in clean samples [16,17]. This can be seen most easily for an isolated interface in a constriction according to the Landauer–Büttiker formula

$$G^{A/B} = \frac{1}{R^{A/B}} = \frac{e^2}{h} \sum_{k_\parallel vs, k'_\parallel v's'} \left| t_{k_\parallel vs, k'_\parallel v's'} \right| = \frac{e^2}{h} \sum_{\mu\mu'} T_{\mu\mu'} \tag{4}$$

where $t_{\mu\mu'}$, $T_{\mu\mu'}$ are the transmission coefficients and probabilities of states $\mu = k_\parallel vs$ at the Fermi energy with (tranverse) wave vector $k_\parallel$ parallel to the interface and band index v. For a ballistic interface $k_\parallel$ and s are conserved during scattering. This expression can be compared with that for a homogeneous point contact of the materials A and B with (Sharvin) conductances $G^A > G^B$. It is clear that any mismatch in the electronic structure will reduce the conductance $G^{A/B} < G^A$.

2.1. Interface resistance

Of interest is the microscopic explanation of the interface resistance parameter $R^{A/B}$ in Eq. (1) and its relation with Eq. (4). The success of the 2CSRM provides the guidance for a quantitative understanding of the experiments. The parameters, which fit so many experiments turn out to be universal for a given material combination. The absence of a measurable dependence on the geometrical parameters d_N and d_F (when everything else is kept the same) is a strong indication that quantum interference terms are negligibly small. For the large thicknesses, which have predominantly been studied experimentally, this is not surprising. But also for significantly exchange-coupled multilayers, quantum well states should not affect significantly transport since disorder causes a large semiclassical background. A semiclassical model, therefore, should be appropriate for all but the cleanest samples with very thin layers. A simple yet efficient *first principles* procedure to incorporate the interfaces comes down to chopping the sample into slices of bulk layers and interfaces which scatter electrons, separated by fictitious non-scattering regions [18]. The bulk layer scattering can be treated in terms of transmission and reflection matrices, modeled in two simple limits; the ballistic limit, in which no scattering occurs during the transmission through the bulk and the diffuse limit in which the scattering is isotropic, which means that the transmitted electrons do not retain any memory of the incident wave vectors. The transmission probabilities for the combined system then follows the semiclassical concatenation of transmission and reflection probability matrices of the resistive elements in series [19,20]. Indeed, the 2CSRM is recovered with interface resistances

$$R^{A/B} = \frac{h}{e^2}\frac{1}{\sum T_{\mu\mu'}} - \frac{1}{2}\left(\frac{1}{G^A} + \frac{1}{G^B}\right). \tag{5}$$

where we have corrected for the spurious geometrical Sharvin resistances [21]. For ballistic bulk layer transmission [18]

$$[R^{A/B}]^{-1} = \frac{e^2}{h} \sum_{\mu\nu} [(\mathbf{I} - T - R)^{-1} T]_{\mu\nu}, \tag{6}$$

which is in fact the 'old' Landauer formula. Both Eqs. (5) and (6) do not contain any parameters and provide a first-principles prescription for the semiclassical interface resistances. They hold not only in the metallic case but should be also valid when the interface is in the tunneling regime. Stiles and Penn [22] confirmed that the expression (Eq. (5)) agrees very well with the solutions of the Boltzmann equation.

Levy et al. [23] recently found strong effects of disorder in the leads on transport through tunnel junctions. Our discussion implies that these effects should be absent in a semiclassical description, which is at odds with the conclusions of Levy et al. Interference effects between impurities and resonance states at the tunnel junction might provide an explanation [24].

2.2. First-principles calculations

The interface resistance has been calculated by first principles for specular interfaces in [18,22,26] for ballistic magnetic domain walls in [25] and diffuse interfaces in [26]. In Table 1 we summarize our results for specular and rough interfaces, the latter modeled as a 50%/50% bilayer alloy, and compare them with available experiments. Remarkable is the different behavior of the Co|Cu as compared with the Fe|Cr interface with respect to the interface roughness: the spin contrast of

the Co|Cu interface transparency is weakly enhanced by disorder, but strongly reduced in Fe|Cr. The message for experimentalists is that in Fe|Cr it should pay off to optimize the epitaxial techniques.

The Boltzmann equation has been solved numerically by Butler et al. [28] for Co|Cu|Co perpendicular spin valves. The constant relaxation time approximation for the bulk materials was used and distribution functions were matched via the transmission and reflection coefficients for specular interfaces. They found results for the interface resistance slightly different from that of [18,26]. Butler et al. find a dependence of the interface resistance on small Cu thicknesses, which appears to contradict the universality of the parameters of the 2CSRM. These corrections are not the small quantum size effects found by Xia et al. [26] and by Tsymbal [27,29], but are purely classical effects due to evanescent terms in the distribution functions. These can be interpreted as the corrections to the assumption of complete isotropy by Schep et al. [18]. The isotropy conditions is expected to be much better fulfilled when interface disorder is taken into account. It is clear that more, also experimental, work is needed to understand transport for very thin layer thicknesses in which the incomplete randomization and the appearance of quantum corrections will cause deviations from the two-channel resistor model.

3. Non-collinear magnetization

Electron transport in devices with non-collinear magnetizations have come into focus by the recent interest in the torque exerted on the magnetization by a spin-polarized injected current [30]. The theories for collinear magnetization mentioned above have been extended to the case in which the magnetizations are not collinear, i.e. not parallel or antiparallel, namely via a magnetoelectronic circuit theory [31], and for CPP spin-valve structures, random matrix theory of transport [32] as well as a direct solution of the diffusion equation in the presence of an external magnetic field [33]. Recently also exchange-biased CPP spin-valves are under scrutiny [43]. We find that these approaches are equivalent and reduce to previous theories in the limit of collinear magnetizations. An interesting point is that [31,32] do not start from the outset with a semiclassical approximation, but derive it from an isotropy assumption, thus put previous more or less ad hoc approaches on firm theoretical foundations.

Table 1
Results of first principles calculation of Eq. (5) [26]

System	Roughness	R_{maj} (fΩm^2)	R_{min} (fΩm^2)
Au/Ag(111)	Clean	0.094	0.094
Au/Ag(111)	2 Layers 50–50 alloy	0.118	0.118
Au/Ag(111)	Exp. [1,2]	0.100 ± 0.008	0.100 ± 0.008
Co/Cu(100)	Clean	0.33	1.79
Co_{hcp}/Cu(111)	Clean	0.60	2.24
Co/Cu(111)	Clean	0.39	1.46
Co/Cu(111)	2 Layers 50–50 alloy	0.41	1.82 ± 0.03
Co/Cu(111)	Exp. [1,2]	0.26 ± 0.06	1.84 ± 0.14
Fe/Cr(100)	Clean	2.82	0.50
Fe/Cr(100)	2 Layers 50–50 alloy	0.99	0.50

3.1. Circuit theory

Transport in hybrid metallic systems can be described by a generalization of Kirchhoff's theory of electronic circuits when parts of the system are not phase-coherently coupled. This approach has been pioneered in [35,36] for electronic networks with superconducting elements. It has recently been adopted also for magnetoelectronic circuits [31], like the Johnson spin transistor [37] or the 4-terminal mesoscopic spin valve of Jedema et al. [12]. For a different approach to the many terminal magnetolectronic circuits, see [38,39]. The circuit theory can be derived from a given Stoner Hamiltonian in terms of the Keldysh non-equilibrium Green function formalism in spin space [34]. The basic physics is provided by splitting up the system into reservoirs, resistors and nodes, where the latter can be real or fictitious (as discussed above). In order to arrive at a useful formalism, an isotropy assumption has to be introduced for the nodes, namely that the electron distributions in the nodes are isotropic, which implies sufficient disorder (or chaotic scattering) to allow for configurational averaging. It does not require any inelastic or dephasing scattering mechanism, although, when happening in the nodes, they will not hurt either. Because the spin-accumulation is not necessarily parallel to the spin-quantization axis, at each node the electron distribution at a given energy ϵ can be denoted as $\hat{f}(\epsilon)$, where the hat denotes a 2×2 matrix in spin-space. The external reservoirs are assumed to be in local equilibrium so that the distribution matrix is diagonal in spin-space and attains its local equilibrium value $\hat{f} = \hat{1} f(\epsilon, \mu_\alpha)$, $\hat{1}$ is the unit matrix, $f(\epsilon, \mu_\alpha)$ is the Fermi–Dirac distribution function and μ_α is the local chemical potential in reservoir α. The direction of the magnetization of the ferromagnetic nodes is denoted by the unit vector $\mathbf{m}_\alpha$. The current through each contact can be calculated as a function of the distribution matrices on the adjacent nodes in terms of 2×2 conductance matrices. The current matrix (for an F|N junctions) reads

$$e\hat{I} = G^{\uparrow}\hat{u}^{\uparrow}(\hat{f}^{F} - \hat{f}^{N})\hat{u}^{\uparrow} + G^{\downarrow}\hat{u}^{\downarrow}(\hat{f}^{F} - \hat{f}^{N})\hat{u}^{\downarrow} - G^{\uparrow\downarrow}\hat{u}^{\uparrow}\hat{f}^{N}\hat{u}^{\downarrow} - (G^{\uparrow\downarrow})^{*}\hat{u}^{\downarrow}\hat{f}^{N}\hat{u}^{\uparrow}, \quad (7)$$

in terms spin-1/2 rotation matrices $\hat{u}^{\uparrow}$, distribution matrices $\hat{f}^{\mathrm{F}}$,$\hat{f}^{\mathrm{N}}$ on ferromagnetic and normal node, the spin-dependent conductances $G^{\uparrow}$ and $G^{\downarrow}$ (which in planar junctions should be corrected as discussed in Section 2)

$$G^{\mathrm{s}} = \frac{e^2}{h}\left[M - \sum_{nm} |r_{\mathrm{s}}^{nm}|^2 \right] = \frac{e^2}{h} \sum_{nm} |t_{\mathrm{s}}^{nm}|^2,$$

and the mixing conductance

$$G^{\mathrm{s},-\mathrm{s}} = \frac{e^2}{h}\left[M - \sum_{nm} r_{\mathrm{s}}^{nm} (r_{-\mathrm{s}}^{nm})^* \right], \tag{8}$$

where r_{s}^{nm}, t_{s}^{nm} are the reflection and transmission coefficients, and M is the number of modes in the absence of reflections. Spin-flips in the contacts have been disregarded. The spin-current conservation law

$$\sum_{\alpha} \hat{I}_{\alpha\beta} = \left(\frac{\partial \hat{f}_{\beta}}{\partial t} \right)_{sf}, \tag{9}$$

then allows computation of the circuit properties as a function of the applied voltages, where $\hat{I}_{\alpha\beta}$ denotes the current from node (or reservoir) α to node (or reservoir) β and the term on the right hand side describes spin-relaxation in the (normal) node. The right hand side of Eq. (9) can be set to zero when the spin current in the node is conserved, i.e. when an electron resides on the node sufficiently shorter than the spin-flip relaxation time τ_{sf}. When the size of the node in the transport direction is smaller than the spin-flip diffusion length $l_{\mathrm{sf}} = \sqrt{D\tau_{\mathrm{sf}}}$, where $D = v_{\mathrm{F}} l_{\mathrm{f}}/3$ is the (3-D) diffusion coefficient then the spin-relaxation in the node can be introduced as $(\partial \hat{f}^{\mathrm{N}}/\partial t)_{\mathrm{sf}} = (\hat{1}\, Tr(\hat{f}^{\mathrm{N}})/2 - \hat{f}^{\mathrm{N}})/\tau_{\mathrm{sf}}$.

Some insight can be gained by re-writing the current and the distribution function in the form of a scalar particle and a vectorial spin contribution, $\hat{I} = (I_0 + \sigma \cdot \mathbf{I}_{\mathrm{s}})/2$, $\hat{f}^{\mathrm{N}} = f_{\mathrm{p}}^{\mathrm{N}} + \sigma \cdot \mathbf{s} \Delta f^{\mathrm{N}}$ and $\hat{f}^{\mathrm{F}} = f_{\mathrm{p}}^{\mathrm{F}} + \sigma \cdot \mathbf{m} \Delta f^{\mathrm{F}}$. The spin current through an F|N interface can then be expanded into different vector components as

$$\begin{aligned} \mathbf{I}_s = \mathbf{m}[&(G^{\uparrow} - G^{\downarrow})(f_{\mathrm{p}}^{\mathrm{F}} - f_{\mathrm{p}}^{\mathrm{N}}) + (G^{\uparrow} + G^{\downarrow})\Delta f^{\mathrm{F}} \\ &+ (G^{\uparrow} + G^{\downarrow} - 2ReG^{\uparrow\downarrow})\mathbf{s} \cdot \mathbf{m} \Delta f^{\mathrm{N}}]\mathbf{s} 2ReG^{\uparrow\downarrow} \Delta f^{\mathrm{N}} \\ &+ (\mathbf{s} \times \mathbf{m}) 2ImG^{\uparrow\downarrow} \Delta f^{\mathrm{N}}. \end{aligned} \tag{10}$$

The vector spin current component perpendicular to the magnetization direction equals the spin-torque exerted by the polarized current on the ferromagnet [30,32].

3.2. Random matrix theory

Waintal et al. [32] have extended the random matrix theory of transport [40] to include non-collinear magnetizations in F|N|F junctions. This paper is focussed on the spin torque, but the physics is essentially the same as for transport in a disordered CPP spin valve with arbitrary magnetization configuration as discussed above. The objects, which are averaged are the scattering matrices of the bulk layer of the normal metal assuming that all members of the ensemble fulfil the symmetry requirements of the problem and are equally probable. The theory is more intricate than in the case of superconducting S|N|S junctions [40], because the averaging has to be carried out over the eigenvalues and eigenvectors. Analytical results can be obtained for the leading term of an expansion into $1/M$, i.e. the inverse of the number of transport channels.

It is easily seen that the analytical relations obtained by Waintal et al. [32] for halfmetallic ferromagnetic elements agree with those from the circuit theory for the symmetric two-terminal device. The general case is less obvious, but by somewhat tedious manipulations a complete equivalence of the final equations for both theories can be proven [41]. We may conclude from Waintal's results that what seemed to be an assumption in the procedure of Schep et al. [18], viz. the semiclassical concatenation, can be *derived* from the isotropy assumption.

Although not yet worked out, Waintal et al.'s approach can be generalized to include quantum corrections, which become important for a small number of channels, as well as many terminal configurations. It is not clear how spin-flip-relaxation processes can be incorporated, which is quite straight-forward for the circuit theory.

3.3. Diffusion equation for non-collinear transport

In some cases the theories above are not sufficient and the spatially dependent distribution has to be evaluated. The spin-polarized electron distribution is characterized by a 2×2 matrix in spin space of the form

$$\hat{f}^{\mathrm{N}}(x) = \begin{pmatrix} f_{\uparrow\uparrow}^{\mathrm{N}}(x) & f_{\uparrow\downarrow}^{\mathrm{N}}(x) \\ f_{\downarrow\uparrow}^{\mathrm{N}}(x) & f_{\downarrow\downarrow}^{\mathrm{N}}(x) \end{pmatrix}. \tag{11}$$

When the size of the system L is larger than the spin diffusion length l_{sf}, $\hat{f}^{\mathrm{N}}(x)$ depends on the position. We have studied transport through an F|N|F device under the condition $l_{\mathrm{f}} \ll l_{\mathrm{sf}}$, where $l_{\mathrm{f}} = v_{\mathrm{F}}(1/\tau + 1/\tau_{\mathrm{sf}})^{-1}$ is the *mean free path*, v_{F} is the Fermi velocity, τ the spin-conserving scattering time and τ_{sf} the spin-flip scattering time [33]. Under the condition $l_{\mathrm{f}} \ll l_{\mathrm{sf}} = \sqrt{D\tau_{\mathrm{sf}}}$, we obtain the generalized diffusion equation in the normal metal

$$\begin{aligned} \frac{\partial^2 \hat{f}^{\mathrm{N}}(x)}{\partial x^2} = &\frac{1}{l_{\mathrm{sf}}^2}\left(\hat{f}^{\mathrm{N}}(x) - \hat{1}\, \frac{Tr(\hat{f}^{\mathrm{N}}(x))}{2} \right) \\ &- \frac{i}{h}\left[\frac{g\mu_B}{2D}(\hat{\sigma} \cdot \vec{B}), \hat{f}^{\mathrm{N}}(x) \right]. \end{aligned} \tag{12}$$

Its solution, with boundary conditions at the interface governed by the conductance matrix, describes e.g. the precession of the spin-accumulation in an applied magnetic field and leads to a physical interpretation of the imaginary part of the mixing conductance [33].

3.4. CPP spin valve

The different approaches described above lead to an analytical expression for the total conductance of CPP spin valves as a function of the angle between the magnetizations of the different ferromagnets θ, when $l_{sf} \gg L$, at zero magnetic field ($\vec{B} = 0$) and for symmetric contacts

$$G^{T}(\theta) = \frac{G}{2}\left(1 - P^2 \frac{\tan^2 \theta/2}{\tan^2 \theta/2 + (|\eta|^2/Re\eta)}\right)$$

where $G = G^{\uparrow} + G^{\downarrow}$, $P = (G^{\uparrow} + G^{\downarrow})/G$,

$$\eta = \frac{2G^{\uparrow\downarrow}}{G}; \quad \frac{|\eta|^2}{Re\eta} = \frac{4|G^{\uparrow\downarrow}|^2}{G^2}\frac{G}{2ReG^{\uparrow\downarrow}} = \frac{2|G^{\uparrow\downarrow}|^2}{GReG^{\uparrow\downarrow}} \tag{13}$$

The angular magnetoconductance reads

$$\frac{G^{T}(\theta) - G^{T}(0)}{G^{T}(\pi) - G^{T}(0)} = \frac{\tan^2 \theta/2}{\tan^2 \theta/2 + (|\eta|^2/Re\eta)}$$

$$= \begin{cases} \sin^2 \theta/2 & \text{for} \quad \eta = Re\eta \to 1 \\ (\mathrm{Re}\eta/|\eta|^2)\tan^2 \theta/2 & \quad\quad \eta \to \infty \end{cases} \tag{14}$$

Balents and Egger [9] arrive at the same result in their study of spin-injection into carbon nanotubes in the non-interacting limit. The electron–electron interaction is found to enhance the mixing conductance.

4. Discussion

Our understanding of the transport properties of the CPP multilayers is semi-quantitative for the parallel aligned and the as grown 'virgin' samples, in which to a good approximation neighboring magnetization vectors are antiparallel. The basis of this understanding is (1) knowledge of the magnetization configuration and (2) the 2CSRM. Bozec et al. [27] claimed to have found evidence for a breakdown of the 2CSRM. However, a recent study with intentionally alloyed bulk layers comes to different conclusions, i.e. that the 2CSRM should remain unchallenged for collinear magnetic structures, be they 'type I' or 'type II', interleaved or separated [42].

The situation of the magnetic-field cycled 'deflowered' samples is more difficult. The experiments of Bozec et al. [27] could be explained by a 'spin-memory' effect caused by spin-flip at the interfaces, which can be incorporated into the 2CSRM [42]. This picture requires that the magnetization at all intermediate fields is random but essentially collinear (except possibly at interfaces). An alternative explanation is Wiser's hypothesis that the angle between the magnetizations of different layers is rotated during magnetization reversal [27]. The transport properties based on this hypothesis can be computed in principle by the generalizations of the 2CSRM to non-collinear transport discussed above, which we may call 'matrix series resistor model'. At the moment the magnetization distribution is not known sufficiently well, but it seems likely that non-collinearity and randomness both play a role. Exchange-biased CPP spin valves appear to be better suited to test the new theories than multilayers [43].

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