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Mesoscopic aspects of the giant magnetoresistance

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Abstract

Microscopic information about electron scattering at heterointerfaces which is relevant for the giant magnetoresistance (GMR) in metallic multilayers can be obtained from measurements carried out in the mesoscopic regime. First-principles calculations of transport through ballistic multilayers demonstrate the importance of taking into account the complicated band structure. The statistics of transport through single disordered interfaces is shown to be non-universal, which means that the fluctuation properties can yield new information on the interface disorder scattering.

1. Mesoscopic transport and the GMR

In recent years consensus has emerged that the scattering which gives rise to GMR in magnetic metallic multilayers occurs predominantly at the interfaces. This is nicely illustrated by transport experiments in the current perpendicular-to-the-interface-plane (CPP) configuration [1–3], in which the (spin-averaged) mean-free-number of traversed interfaces in Co/Cu multilayers [4] is 1.4 (or 4.4 when the reduction of the number of conducting channels found by band structure calculations [10] is taken into account) although the electronic mean free path in the bulk of the layers is several tens of nanometers. However, in spite of this knowledge virtually nothing is known about what happens on a microscopic scale when an electron is incident upon a disordered interface. The theoretical models used up to now [5,3] are essentially only straightforward generalizations of the venerable Fuchs model [6]! In the context of the GMR effect this means that (i) we do not know *a priori* how to choose materials which give large GMR effects, and (ii) no recipe exists on how to prepare the interfaces to maximize the effect for a given multilayer.

The purpose of our theoretical work [7–12] is to understand the microscopic nature of the electron scattering phenomena at heterointerfaces and multilayers in the mesoscopic regime. We not only hope to find new physical effects, but also to obtain a better understanding of the factors which control the GMR in macroscopic samples, and which cannot be identified by other means due to insufficient characterization or quality of the sample morphology. Two different and in principle independent regimes are of interest, namely the *ballistic* regime, where the mean-free path is larger than the spatial extent of the region of the potential drop (the 'sample'), or the

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phase-coherent regime, where the phase-coherence length is larger than the sample dimension. Both regimes can be realized in metallic point contacts with nanometer dimensions [13].

2. Ballistic multilayers

We have carried out first-principles band structure calculations of the ballistic transport properties of a number of magnetic metallic multilayers [10,11]. No empirical parameters or other phenomenological input are used and the effects of the complex electronic structure, such as the s–d hybridization, is fully taken into account. The hybridization has been shown to make an important contribution to the giant magnetoresistance (MR) effect in Co/Cu superlattices [10]. We investigated the MR in Fe/Cr in the same way and found some interesting differences compared to the Co/Cu system [11]. In contrast to Co/Cu the minority spin has the larger conductance and the MR in the CIP (current-in-plane) configuration remains significant for relatively wide spacer layers. Last but not least a larger MR of up to 200% is calculated in the CPP geometry. When the magnetic and non-magnetic layer thicknesses are varied we find pronounced quantum size effects in the MR. These results will be explained in more detail by Schep et al. [11].

We want to stress that an experimental realization of the ballistic regime is of utmost importance for progress in the field. Although the predictive power of first-principles band structure calculations is well documented in other fields, the agreement of experiment and theory for dc transport properties of disordered multilayers is not yet convincing [14]. Any progress in disordered samples should be based on a good understanding of the ordered systems. In spite of the absence of experimental verification we believe that these calculations are a useful instrument for screening combinations of materials for their suitability in magnetoresistive device applications.

However, a large GMR effect in the ballistic regime is a necessary, but not a sufficient condition for a good material (combination), because in practice the interfaces are not perfect. Although this topic is still controversial, some interface scattering almost certainly has a beneficial effect for the MR in the CIP configuration. For Co/Cu this seems to hold also for the CPP configuration, where the theoretical ballistic GMR ratios are of the same order of magnitude, but smaller than the experimental ones. For Fe/Cr the situation is not yet fully established, since the ballistic GMR ratios are larger than the experimental ones obtained by Gijs et al. [12]

3. Disordered interfaces

In a conventional transport experiment there is only one observable (or two in the case of the GMR), namely the conductance, which is not sufficient to establish a certain model. However, recently we found [12] that the statistical transport properties of phase-coherent interfaces depend sensitively on the details of the scattering potentials (in contrast to the so-called universal conductance fluctuations in diffusive wires [15–17]). This provides additional and possibly crucial experimental information for unravelling the interface structure and scattering. In the following we discuss from a theoretical point of view the new information which can be obtained by studying the transport properties of single metallic interfaces in the mesoscopic regime where the electronic wave function is fully phase coherent.

The statistical properties of transport in disordered mesoscopic conductors is a very active field of theoretical solid state physics [17]. One of the phenomena of central interest are the statistical fluctuations $\delta G = \{\langle G^2\rangle - \langle G\rangle^2\}^{1/2}$ of the average conductance $\langle G\rangle$ denoting the ensemble average over impurity configurations by $\langle \cdots \rangle$. In diffusive phase-coherent systems these fluctuations are universal, i.e. independent of sample size and details of the disorder [15,16]. Transport theory of mesoscopic systems is based on Landauer's formula for the conductance G, which for zero magnetic field and non-magnetic systems reads

$$G = \frac{2e^2}{h}\mathrm{Tr}\,\boldsymbol{T} = \frac{2e^2}{h}\sum_n T_n, \tag{1}$$

where T_n are the eigenvalues of the transmission matrix $\boldsymbol{T}$. The quantities of interest are the distribution function of the eigenvalues T_n of the transmission matrix,

$$P(T) = \left\langle \sum_n \delta(T - T_n) \right\rangle, \tag{2}$$

and the correlation function,

$$P(T, T') = \left\langle \sum_n \delta(T - T_n) \sum_m \delta(T' - T_m) \right\rangle \tag{3}$$

Beenakker [18] emphasized that the availability of these functions allows direct calculation of various physical properties and their variances, such as shot noise power and the transport properties of N(ormal)/S(uperconducting) and S/N/S Josephson junctions. In general, for a property a described by a linear statistic $a(T)$,

$$\langle a \rangle = \left\langle \sum_n a(T_n) \right\rangle = \int \mathrm{d}T\, a(T) P(T), \tag{4}$$

and $\mathrm{Var}(a) = \langle a^2 \rangle - \langle a \rangle^2$, with

$$\langle a^2 \rangle = \int \mathrm{d}T\, \mathrm{d}T'\; a(T) a(T') P(T, T'). \tag{5}$$

Random matrix theory (RMT) of transport has been invoked to explain the universality [19]. The distribution function of the transmission matrix eigenvalues ('levels') of sufficiently random systems are interpreted in terms of classical fictitious charges in one dimension which repel each other with the two-dimensional Coulomb interaction. The universality of the conductance fluctuations is explained by the spectral rigidity caused by the level repulsion, which reflects the negligible weight of highly symmetrical matrices in the maximum entropy ensemble average [20]. While fascinating from a fundamental point of view, universality could be a nuisance for the materials scientist, because it prohibits any engineering of the transport properties. Furthermore, the measured conductances only depend on a single mean free path parameter,whereas the fluctuations do not contain any information at all. Fortunately, this is not the case for transport through a single disordered interface.

The present paper is devoted to the theory of transport through a disordered region which is much shorter (or thinner) than the average distance between scatterers and much wider than the Fermi wavelength, i.e. without appreciable effects of size quantization, in an otherwise ballistic constriction or wire. Physically this model represents, for example, a (not too) rough metallic heterointerface as relevant for the CPP configuration [1,2]. The microscopic theory is quite complex, and in spite of what we said above about the necessity to take the full electronic structure into consideration, we have to return to a model of free electrons and short-range impurity potentials [8], keeping in mind that not all parameters are well determined. The elements of the transmission matrix $\boldsymbol{T} = \boldsymbol{t}\boldsymbol{t}^{\dagger}$ are labeled by the components $\boldsymbol{k}_{\parallel}$ of the momentum, parallel to the interface, of the in- and outgoing planes waves. The transmission coefficients $\boldsymbol{t}$ can be expanded as

$$\boldsymbol{t} = \sum_{N=0}^{\infty} (-\mathrm{i}\boldsymbol{\Gamma})^N. \tag{6}$$

$$\Gamma_{k_{\parallel}, k'_{\parallel}} \equiv \frac{m^*}{A\hbar^2} \sum_{\alpha} \gamma_{\alpha}\, \mathrm{e}^{-\mathrm{i}(k_{\parallel} - k'_{\parallel})\rho_{\alpha}} \frac{1}{\sqrt{k_{\perp} k'_{\perp}}} \tag{7}$$

depends on the scattering centers located randomly at $\boldsymbol{\rho}_{\alpha}$ on the interface with potentials $\gamma_{\alpha} = \pm\gamma$, whose ensemble average is assumed to be zero. A is the interface cross section and the perpendicular component $k_{\perp}$ is defined in terms of the Fermi wave vector k_{F} as $k_{\perp}^2 = k_{\mathrm{F}}^2 - |\boldsymbol{k}_{\parallel}|^2$. A noteworthy feature of the present model is the absence of the coordinate normal to the interface. Of crucial importance are the Ward identities $\boldsymbol{t}\boldsymbol{t}^{\dagger} = (\boldsymbol{t} + \boldsymbol{t}^{\dagger})/2$ and $\boldsymbol{t}\boldsymbol{t} = (1 + \gamma\partial/\partial\gamma)\boldsymbol{t}$, which can be proven by direct substitution of Eqs. (6),(7) and which hold only for the single interface. By expressing the δ-function in Eq. (2) as a Fourier integral, expanding the exponent $\mathrm{e}^{\mathrm{i}qT}$ as a power series in $\boldsymbol{T}$, and repeatedly using the Ward identities, we derive

$$P(T) = \int \frac{\mathrm{d}q}{2\pi}\, \mathrm{e}^{-\mathrm{i}qT} \left(g_0 + \sum_{n=1}^{\infty} \frac{(\mathrm{i}q)^n}{n!} f_{n-1}\left(\eta \frac{\partial}{\partial \eta} \right) \langle g(\eta) \rangle \right), \tag{8}$$

where

$$f_n(N) = \binom{N+n}{n}$$

is a polynomial in N, $g_0 = \mathrm{Tr}\, \boldsymbol{I} = Ak_{\mathrm{F}}^2/(4\pi)$ is the number of modes, and $g(\eta) = \mathrm{Tr}\, \boldsymbol{T}(\eta)$ denotes the dimensionless conductance as a function of the squared scattering potential $\eta = \gamma^2$. Configurational averages can be calculated most conveniently by Green's function methods [8]:

$$\langle T_{k_\parallel, k'_\parallel} \rangle = \delta_{k_\parallel, k'_\parallel} \Re \frac{1}{1 + \mathrm{i}\left(m^*/\hbar^2 k_\perp\right)\Sigma}, \tag{9}$$

where Σ is the irreducible self-energy, and $\Re$ denotes the real part.

The correlation function Eq. (3) can be treated analogously by operating with the differential operators on

$$g(\eta)\ g(\eta') = \tfrac{1}{2}\Re\left[\mathrm{Tr}\ t(\eta)\ \mathrm{Tr}\ t(\eta') + \mathrm{Tr}\ t(\eta)\ \mathrm{Tr}\ t^\dagger(\eta')\right], \tag{10}$$

where the Ward identities have again been used. The vertex correction in the configurational average of Eq. (10) contains all information about the fluctuations.

All results up to now are exact for the given model. In particular they are not limited to weak scattering potentials. In practical calculations, expressions for the self-energy and the vertex correction have to be chosen, from which all statistical properties can be computed. We are now in a position to discuss two selected phenomena, i.e. the importance of non-Born scattering on the level density and the absence of an appreciable long-range level repulsion.

The single-site (CPA) approximation to the self-energy [8] is valid when the scattering potential is weak, but also for strong scattering potentials, provided the density of scatterers n_{IR} is small. After some algebra Eq. (8) reduces to

$$P_{\mathrm{S}}(T) = g_{\mathrm{S}}(\infty)\,\delta(T-1) + g_0 \frac{T}{1-T} \frac{2\eta_{\mathrm{B}}^2 T}{1 - T(1+\eta_{\mathrm{B}}/\eta_\infty)^2}, \tag{11}$$

for $T \leqslant T_{\max}^{\mathrm{S}} = 1/[1 + \eta_{\mathrm{B}} + \eta_{\mathrm{B}}/\eta_\infty]$, and zero otherwise. Here $\eta_{\mathrm{B}} = (m^*/\hbar^2)^2 n_{\mathrm{IR}} \gamma^2/(2\pi)$, $\eta_\infty = 2\pi n_{\mathrm{IR}}/k_{\mathrm{F}}^2$, and $g_{\mathrm{S}}(\infty)$ is the conductance in the limit of strong scattering potentials [8]. In the weak scattering limit ($\eta_{\mathrm{B}} \ll 1$ and $\eta_\infty \to \infty$) the Born approximation is recovered and $g_{\mathrm{S}}(\infty)$ vanishes (see Fig. 1). The physical consequences become evident in Fig. 2, where the averages of three transport properties are plotted for the intermediate regime as a function of the impurity density η_∞ and a fixed $\eta_{\mathrm{B}} = 0.3$. Small η_∞ correspond to strong scattering potentials. Noteworthy is the drop of the conductance of the N/S junction below the normal conductance in the Born scattering limit, a direct consequence of the lack of highly transmitting states. Measuring the conductance and the shot noise power of a single disordered interfaces with and without a superconducting contact contains important information on the strength and density of the scattering centers.

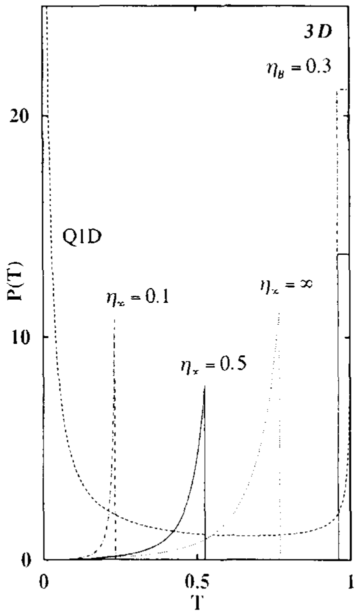

Fig. 1. Level density distribution as calculated in the single-site approximation Eq. (11) for constant $\eta_{\mathrm{B}} = 0.3$ and different values of $\eta_\infty = 2\pi n_{\mathrm{IR}}/k_{\mathrm{F}}^2$. The dashed line labeled Q1D denotes the bimodal distribution of the transmission matrix eigenvalues in long wires [22]. The blocks on the right represent the integrated strength of the δ-functions at $T = 1$.

The level correlation has been calculated in Ref. [12] from Eq. (3) for a two-dimensional 'impurity necklace' in the Born approximation. The results for 3D systems are expected to be quantitatively, but not qualitatively different. δG turns out to be strongly non-universal, scaling like $\sqrt{G}$. This conspicuous breakdown of random matrix theory for a disordered system can be traced to the absence of a long-range level repulsion which suppresses the fluctuations in diffusive systems [12]. The fluctuations also depend sensitively on the nature of the impurity scattering

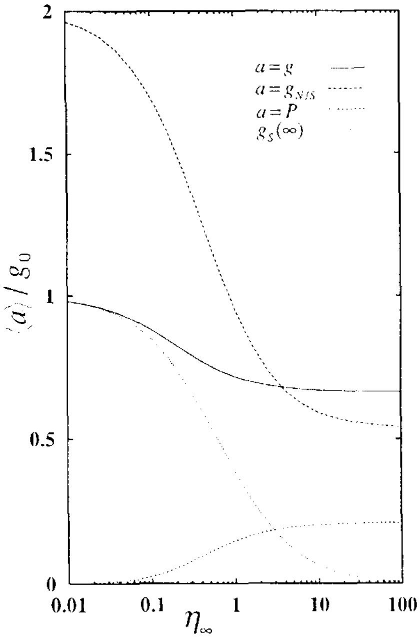

Fig. 2. Average transport properties $\langle a \rangle$ (in units of g_0) through a disordered interface as calculated in the single site (CPA) approximation to the self-energy as a function of η_∞ and a constant $\eta_B = 0.3$. Normal conductance $a(T) = T$ (full curve), conductance of an N/S junction $a(T) = 2T^2/(2-T)^2$ (long dashes), shot noise power $a(T) = T(1-T)$ (short dashes). The dotted curve represents the number of completely transmitted states $g_S(\infty)$.

potentials. Vice versa, we may conclude that the conductance fluctuations contain a lot of information on the scattering potentials. All other transport properties are also non-universal and provide independent information on the 'black box' of the disordered interface. Experimental determination of not only the average conductances, but also the fluctuations of the transport properties through single interfaces in the phase-coherent regime can provide microscopic information on the scattering processes responsible for the GMR effect, which is not accessible otherwise. Theoretically, the present study has to be expanded to include effects of spin, potential steps or barriers, and evanescent states. An interesting consequence of a step potential in the specular limit is a finite shot noise power, but vanishing conductance fluctuations. The analytical calculations can be tested by recursive Green's function calculations [21]. Of particular interest is the double interface configuration (CPP spin valve), which should give important additional insights into the fundamental transport theory of the GMR effect and the level repulsion concept in phase-coherent transport.

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