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1997 J. Phys.: Condens. Matter 9 7135

(http://iopscience.iop.org/0953-8984/9/34/007)

J. Phys.: Condens. Matter **9** (1997) 7135–7140. Printed in the UK PII: S0953-8984(97)82154-6

Exchange coupling and ballistic current-perpendicular-to-plane giant magnetoresistance in magnetic trilayers: mutual intercorrelations

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Received 25 February 1997, in final form 13 June 1997

Abstract. It is shown that the current-perpendicular-to-plane giant-magnetoresistance (CPP-GMR) oscillations, in the ballistic regime, are strongly correlated with those of the exchange coupling (J). Both the GMR and J are treated *on an equal footing* within a rigorously solvable tight-binding single-band model. The strong correlation consists in an asymptotic sharing of the same period, determined by the Fermi surface, and oscillations with varying spacer thickness predominantly in *opposite phases*.

The *oscillatory behaviour* of many physical phenomena of magnetic multilayer systems manifests itself in the most spectacular way as a function of spacer thickness, but the magnetic layer thickness is relevant too [1–3]. The most widely studied oscillatory phenomena are those connected with either (i) the exchange coupling (J) or (ii) the so-called giant magnetoresistance (GMR) (see references [3] and [4] for a review of the current understanding of these phenomena). The exchange coupling is of quantum nature, and is well understood in terms of such theoretical approaches as RKKY-type theory [3], the theory of quantum well states, [5], the tight-binding model [6], and the free-electron-like one [7]. From these approaches, as well as experimental results [8] and *ab initio* band-structure calculations [9, 2], consensus emerges that the oscillation periods of J are determined by certain extremal spanning vectors of the spacer Fermi surface. As regards the GMR, according to the two-spin-channels model, one expects a strong influence of the exchange coupling (responsible for the mutual orientation of the magnetization of ferromagnetic slabs) on the resistivity. This is in fact the case, due to the obvious spin asymmetry. In the case of the parallel configuration there is one spin direction (dependent on the density of states at the Fermi energy) for which the conduction electrons are weakly scattered in all of the magnetic layers, and the shunting of the current by this low-resistivity spin channel reduces the total resistivity. For the antiparallel configuration, the carriers are weakly scattered only in every other magnetic slab, and consequently the resistivity is less effectively reduced.

The GMR can be easily measured if the relative spontaneous orientation of the magnetizations of the magnetic slabs is antiparallel (negative J), since then we simply have GMR $= (R(0) - R(H))/R(0)$, where H is the magnetic field necessary to switch to the parallel orientation; but the GMR remains well defined in the opposite case, too. While the latter case presents no problem for a theoretical treatment, it requires fairly sophisticated

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handling (atomic engineering) in order to stabilize the antiparallel orientation by pinning one of the ferromagnetic slab magnetizations [10].

Although the GMR in general is not of quantum origin, and contains some ingredients which are hard to control (defects, impurities, surface and interface roughness, etc), there is one contribution, due to reflections of electrons from quantum well barriers, which is of the same origin as the exchange coupling. This *quantum contribution* has already been shown to be quite substantial; see [11–13].

The aim of the present paper is to confront the GMR oscillations in the ballistic regime [14, 12, 13], where only the quantum contribution appears, with those of the exchange coupling. For the first time, as far as the authors are aware, both quantities are treated simultaneously on an equal footing without any approximations, by precise numerical computations.

In fact, in spite of there being plenty of publications on the GMR and J, there has been, to our knowledge, only one theoretical attempt, in reference [7], devoted to a detailed comparison of the two quantities: the authors of reference [7] have used a free-electron-like model, compared the J-behaviour with that of the *current-in-plane* (CIP) GMR, and found that the CIP-GMR assumes maxima for the *parallel* orientation. In contrast, in our calculation, which concentrates on the *current-perpendicular-to-plane* (CPP) GMR in the ballistic limit, i.e. without impurities, the maxima in the GMR arise for the *antiparallel* orientation. Although the precise reason for this discrepancy is not yet clear, one should note in the present context that in [7] the relevant quantities could not be treated on an equal footing, since some inconsistency was unavoidable as a result of taking into account electron scattering by impurities.

In the present paper we therefore put emphasis on selecting the above-mentioned CPP-GMR component *of purely quantum origin*, which can be directly compared with the exchange coupling, and, in principle, measured in the ballistic regime [15]. On the one hand, the ballistic conductance mechanism has been well known for many years now [16], and, on the other hand, ballistic point contacts have already been fabricated [15]. So one can expect that ballistic transport in metallic multilayers will be studied in the near future, although, admittedly, the present experiments deal with the diffusive regime.

In the following, we adopt the rigorously solvable tight-binding single-band model Hamiltonian

$$H_\sigma = \sum_{i,j} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} + \sum_{i} V_\sigma(\boldsymbol{i}) c^\dagger_{i,\sigma} c_{i,\sigma} \tag{1}$$

with t being the nearest-neighbour hopping integral ($|t|$ is the energy unit), and $V_\sigma(\boldsymbol{i})$ being the spin-dependent atomic potential. The systems under consideration are trilayers of the type $n_f\mathrm{F}/n_s\mathrm{S}/n_f\mathrm{F}$, where n_f (n_s) stands for the number of ferromagnetic (non-magnetic spacer) monolayers in the perpendicular z-direction. The ferromagnetic slabs are magnetized either parallel or antiparallel to each other. Since the systems are infinite in the (x, y)-plane and the potentials V_σ are only z-dependent, the eigenvalues of the Hamiltonian (1) for simple cubic lattices (with the lattice constant $= 1$) are simply

$$E(\boldsymbol{k}_\parallel, \tau) = \epsilon_\perp(\tau) - 2(\cos k_x + \cos k_y) \tag{2}$$

where the $\epsilon_\perp$ are the eigenvalues, labelled with τ, of a tridiagonal matrix of rank $2n_f + n_s$ (with free boundary conditions in the z-direction). The exchange splittings of the ferromagnetic films have been introduced by taking spin-dependent atomic potentials V_σ outside the spacer. Additionally we have assumed a perfect matching of the minority bands throughout the whole system by putting $V_\downarrow = 0$.

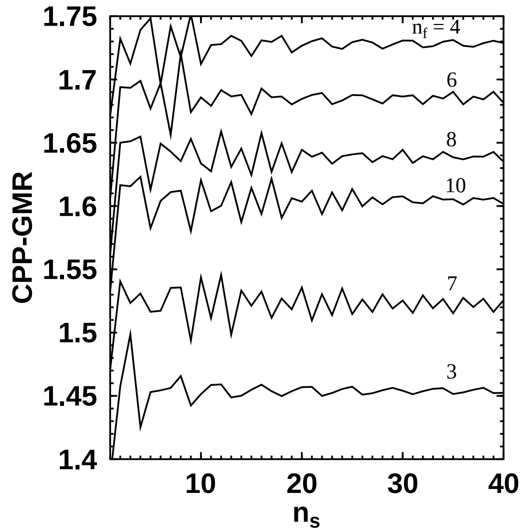

Figure 1. The CPP-GMR of the systems $n_f\mathrm{F}/n_s\mathrm{S}/n_f\mathrm{F}$ (where n_f and n_s are the numbers of ferromagnetic and non-magnetic spacer monolayers, respectively). The majority-spin electrons have the potentials $V_\uparrow = -1.8$ in the ferromagnets (all other potentials are 0); $E_F = 2.5$.

The exchange coupling is then calculated in the following way [1, 17]:

$$\Omega = \sum_{\boldsymbol{k}_\parallel,\tau}[E(\boldsymbol{k}_\parallel,\tau) - E_F]\theta(E_F - E(\boldsymbol{k}_\parallel,\tau)) \tag{3}$$

$$J = \Omega_\uparrow^{\uparrow\downarrow} + \Omega_\downarrow^{\uparrow\downarrow} - \Omega_\uparrow^{\uparrow\uparrow} - \Omega_\downarrow^{\uparrow\uparrow} \tag{4}$$

i.e. J is the difference of the thermodynamic potentials for antiparallel- and parallel-magnetized configurations. The summation in (3) has been performed very accurately by means of the *special-k-points* method [18].

At the same time—and on exactly the same footing—we compute the CPP-GMR in the ballistic limit using the method of our recent paper [13]. This method uses the Kubo formula, and applies an extremely accurate recursion Green's function algorithm to trilayer systems sandwiched between semi-infinite ideal lead wires. The method, based on references [19, 20] and modified by us in reference [13], is rigorous. Due to this modification we have been able to reduce the problem to one dimension, making it possible to study systems thick enough to manifest the important asymptotic trends.

The GMR is defined by

$$\mathrm{GMR} = \frac{\Gamma_\uparrow^{\uparrow\uparrow} + \Gamma_\downarrow^{\uparrow\uparrow}}{\Gamma_\uparrow^{\uparrow\downarrow} + \Gamma_\downarrow^{\uparrow\downarrow}} - 1 \tag{5}$$

where Γ is the conductance, and the superscripts and subscripts indicate the relative orientation of the magnetization, and the electron spin, respectively.

Thus we can now directly compare results for the exchange coupling and for the ballistic CPP-GMR, both obtained at the same level of accuracy and for the same model.

In figure 1 we present some typical plots of the GMR versus n_s for different magnetic slab thicknesses (n_f). What is easy to see is that for small n_f the curves have a regular quasiperiodic behaviour which seems to be disturbed for n_f greater than, say, 6. Before we explain this situation, let us briefly recall that in the asymptotic limit of large n_s one expects

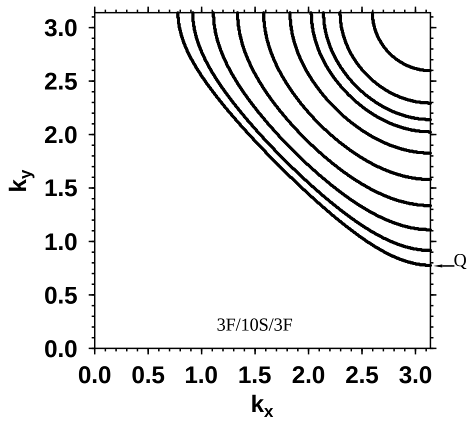

Figure 2. The Fermi surface of the systems under consideration consists of $\epsilon_\perp$-constant energy contours with occupied states inside, where $\epsilon_\perp$ fulfils: $\epsilon_\perp - 2(\cos k_x + \cos k_y) = E_F$. The arrow indicates the extremal spanning vector Q for the 3F/10S/3F system (in the *parallel* configuration, with $E_F = 2.5$ and $V_\uparrow = -1.8$).

a quasiperiodic behaviour of the exchange coupling with a period depending exclusively on the Fermi energy which (for a given lattice structure) determines extremal spanning vectors of the spacer Fermi surface. Figure 2 exemplifies this for the 3F/10S/3F system with $E_F = 2.5$. The Fermi surface has the form of $\epsilon_\perp$-constant contours with occupied electronic states inside. The arrow indicates the spanning vector with the following components: $[k_x = \pi,\ k_y = Q = 0.774,\ \epsilon_\perp = 1.929]$. We quote the numerical values to show that for a relatively small system with 16 monolayers in the z-direction, $\epsilon_\perp$ is already close to the asymptotic value 2, i.e. $k_z = \pi$. Thus, asymptotically, for $n_s \to \infty$, when the equivalence of all of the directions is restored, and k_z becomes a good quantum number, one gets the spanning vectors $[\pi, Q, \pi]$, and, by symmetry, $[\pi, \pi, Q]$, i.e. the oscillation period $\lambda = \pi/Q \approx 4$. Incidently, it is very easy to predict the period length in this limit, by minimizing with respect to k_x and k_y the following function:

$$k_z(k_x, k_y, E_f) = \arccos(-E_f/2 - \cos k_x - \cos k_y) \tag{6}$$

which gives $Q = k_z^{extr}$ for $(k_x, k_y) = (0, 0)$, $(\pm\pi, 0)$, $(0, \pm\pi)$, and $(\pm\pi, \pm\pi)$. Another fact worth mentioning is that the influence of the magnetic slab thickness on the J-oscillations only leads to some phase shifts, without actually changing the period length [3, 17].

In figure 3 we show both the GMR and J for $n_f = 3$ and $V_\uparrow = -1.8$, and find fairly well correlated oscillations with the same period $\lambda \approx 4$, consistent with the strictly calculated Fermi surface and the sketchy estimations above. It turns out that this conclusion holds also for the other curves in figure 1, but to see this one has to take a closer look at them, and allow for greater values of n_s to select the asymptotic trend. This has been made clear in figures 4 and 5 for $n_f = 7$ and 5, with a period of about 10 in the latter case. It is easily seen that the GMR does share with the exchange coupling the long period of oscillations, but has predominantly an *opposite phase* [21], in the sense that for negative (positive) J it takes larger (smaller) values than its asymptotic value. This coincidence would be hardly visible for small n_s until the asymptotic behaviour develops, and is partially obscured by the superposition of some short-period oscillations of the GMR of non-RKKY nature [12, 13]. It is worth mentioning in this context that our models differ from those of [12] in two respects: (i) our magnetic sublayers are finite whereas those of [12] are semi-infinite; and

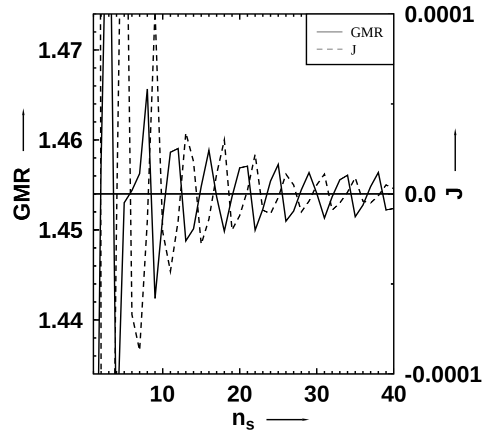

Figure 3. The GMR (solid line) and *exchange coupling* (J) (dashed line) versus the spacer thickness, for $n_f = 3$, $E_F = 2.5$ and $V_\uparrow = -1.8$.

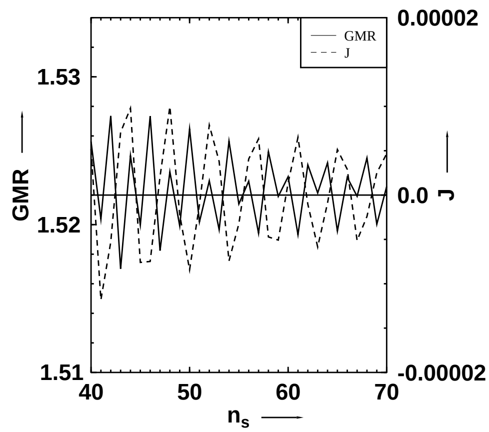

Figure 4. As figure 3, but with $n_f = 7$ and for higher values of n_s, plotted to reveal the asymptotic trend of the oscillations.

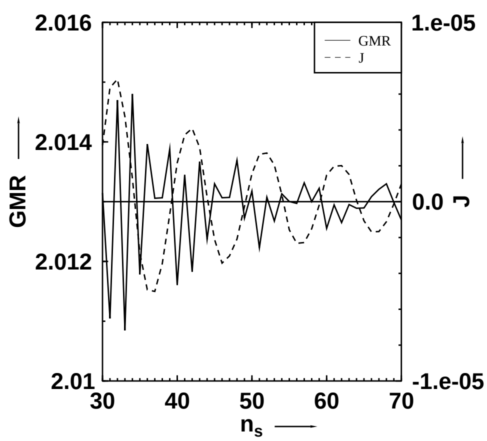

Figure 5. As figure 4, but with $n_f = 5$, $E_F = 2.1$, and $V_\uparrow = -2$.

(ii) we use the (negative) potential wells for majority-spin electrons in the magnetic layers (and the vanishing potentials elsewhere) instead of (positive) potential barriers for minority-spin electrons. The characteristic beats of the GMR (resulting from the superposition of two periods) reported in [12] occur in our model, too. They are very pronounced as a function of the ferromagnetic slab thickness in our case [13], but a second non-RKKY CPP-GMR period appears also with the varying spacer thickness, provided that the magnetic slabs are thick enough (figures 4 and 5 in contrast to figure 3). Our results concerning the CPP-GMR are valid in the ballistic regime, which implies that the impurity concentration must be small enough in relation to the ballistic electron mean free path. However, we would like to stress that, according to our previous study, reference [13], some moderate interface roughness could only wash out the short-wave oscillations without essentially modifying the longer periods of the order of $\lambda \gtrsim 4$. The CIP-GMR is known to be much more sensitive to imperfections than the CPP-GMR (see [20]); thus the striking differences in the oscillation phases between our findings and those of [7] should most probably be ascribed to the role of impurities. A detailed comparison of the CPP- and CIP-GMR, treated consistently with the underlying exchange coupling, will be a matter for our future research.

In conclusion, we have carried out numerical studies of a rigorously solvable tight-binding single-band model, treating the CPP-GMR and the exchange coupling J on an equal footing, by avoiding impurities, and found that, asymptotically, the two quantities not only share the same oscillation period (consistent with the Fermi surface topology), but also have predominantly opposite phases.

Acknowledgments

This work has been carried out under the bilateral project DFG/PAN 436 POL (UK, SK), and the KBN grants No 2 PO3B 099 11, 2P 03B 165 10 (SK), and 2P 302 005 07 (MZ). We also thank the Poznań and Regensburg Computer Centres for computing time.

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