Exchange coupling and current-perpendicular-to-plane giant magneto-resistance of magnetic trilayers. Rigorous results within a tight-binding single-band model.

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Abstract

It is shown that the current-perpendicular-to-plane giant magneto-resistance (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 equal footing within a rigorously solvable tight-binding single-band model. The strong correlation consists in sharing asymptotically the same period, determined by the spacer Fermi surface, and oscillating with varying spacer thickness predominantly in opposite phases.

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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. The most widely studied oscillatory phenomena are those connected with either the exchange coupling ($J$) or the so called giant magneto-resistance (GMR) (see Refs. 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 like: RKKY-type theory, quantum well states, tight-binding
model\cite{7}, and free-electron-like one\cite{7}. From these approaches as well as experimental results\cite{8} and \textit{ab initio} band structure calculations\cite{9}, consensus emerges on 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-spins 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. The anticipated trend would be to relate the antiparallel (parallel) orientation with maxima (minima) of GMR. The GMR can be easily measured if the relative spontaneous orientation of the magnetizations of the magnetic slabs is antiparallel (negative $J$), since then simply $\text{GMR} = (R(0) - R(H))/R(0)$, where $H$ is the magnetic field necessary to switch to the parallel orientation; but GMR remains well defined in the opposite case, too. While the latter case makes no problem for a theoretical treatment, it requires pretty sophisticated handling (atomic engineering) in order to stabilize the antiparallel orientation by pinning one of the ferromagnetic slab magnetizations\cite{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 \textit{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 been studied and shown to be quite substantial both by \textit{first principles} computations\cite{11} and model calculations\cite{12,13}. The aim of the present paper is to confront the GMR oscillations in the ballistic regime\cite{12,13}, where only the quantum contribution appears, with those of the exchange coupling. Both quantities are treated on equal footing without any approximations, by precise numerical computations.

It is interesting that in spite of plenty of publications on GMR and $J$, there has been, to our knowledge, only one theoretical attempt\cite{7} devoted to a detailed comparison of both quantities. The authors of Ref. 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. That study could not treat, however, the relevant quantities on equal footing since some inconsistency was unavoidable as a result of
taking into account electron scattering by impurities. As we will see below, in our model the maxima, for the current-perpendicular-to-plane (CPP) GMR arise for the antiparallel orientation.

In the present letter we 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. We adopt the rigorously solvable tight-binding single-band model Hamiltonian

$$ H_\sigma = \sum_{\vec{i},\vec{j}} t_{i,j} c_{\vec{i},\sigma}^\dagger c_{\vec{j},\sigma} + \sum_{\vec{i}} V_\sigma(\vec{i}) c_{\vec{i},\sigma}^\dagger c_{\vec{i},\sigma}, $$

(1)

with $t$ being the nearest-neighbour hopping integral ($|t|$ is the energy unit) and $V_\sigma(\vec{i})$ – the spin-dependent atomic potential. The systems under consideration are trilayers of the type $n_f F/n_s S/n_f F$, where $n_f$ ($n_s$) stands for the number of the 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 $V_\sigma$ are only $z$-dependent, the eigenvalues of the Hamiltonian (1) for simple cubic lattices (with the lattice constant = 1) are simply:

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

(2)

where $\epsilon_{\perp}$ are the eigen-values, labeled by $\tau$, of a tridigonal 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 $V_\sigma$ outside the spacer. Additionally we have assumed a perfect matching of the minority bands in the whole system by putting $V_\downarrow = 0$. The exchange coupling is then calculated in the following way:

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

(3)

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

(4)
i.e. $J$ is the difference of the grand-canonical thermodynamic potentials for antiparallelly and parallelly magnetized configurations. The summation in (3) has been performed very accurately by means of the *special k-points method*\textsuperscript{17}.

The way we compute the CPP-GMR is the same exact one as in our recent paper\textsuperscript{13}. It uses the Kubo formula and applies an accurate recursion Green’s function method to trilayer systems sandwiched between semi-infinite ideal lead wires. The method, based on Refs. 18,19 and modified by us in Ref. 13, is rigorous. The GMR is defined by

$$\text{GMR} = \frac{\Gamma_{\uparrow\uparrow}^{\uparrow\uparrow} + \Gamma_{\downarrow\downarrow}^{\uparrow\uparrow}}{\Gamma_{\uparrow\downarrow}^{\downarrow\uparrow} + \Gamma_{\downarrow\uparrow}^{\downarrow\uparrow}} - 1,$$

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

In Fig. 1 we present some typical plots of GMR vs. $n_s$ 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 puzzling situation let us briefly remind that in the asymptotic limit of large $n_s$ one expects 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. Fig. 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 $Q$ with the following components $[k_x = \pi, k_y = Q = 0.774, \epsilon_\perp = 1.929]$. We quote the numerical values to show that already for a relatively small system with 16 monolayers in the $z$-direction $\epsilon_\perp$ is close to the asymptotic value 2, i.e. $k_z = \pi$. Thus, asymptotically, for $n_s \to \infty$, when the equivalence of all the directions is restored and $k_z$ becomes a good quantum number, one gets spanning vectors $[\pi, Q, \pi]$ and, by symmetry, $[\pi, \pi, Q]$, i.e. the oscillation period $\lambda = \pi/Q \approx 4$. Incidentally, it is very easy to predict a period length in this limit, by minimizing with respect to $k_x$ and $k_y$ the following function:

$$k_z(k_x, k_y, E_f) = \arccos(-E_f/2 - \cos k_x - \cos k_y),$$

(6)
which gives $Q = k_z^{extr}$ for $(k_x, k_y) = (0, 0), (\pm \pi, 0), (0, \pm \pi), (\pm \pi, \pm \pi)$. 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.34

In Fig. 3 we show both GMR and $J$ for $n_f = 3$ and $V_1 = -1.8$ and find pretty well correlated oscillations with the same period 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 Fig. 1, but to see it one has to take a closer eye at them and allow for greater values of $n_s$ to select the asymptotic trend. That has been made clear in Figs. 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, in the sense that for negative (positive) $J$ it takes larger (smaller) values than its asymptotic value. This coincidence is hardly visible for small $n_s$ until the asymptotic behaviour develops, and is partially obscured by the superposition of some short period oscillations of GMR of non-RKKY nature.12-13

In conclusion, we have carried out numerical studies of a rigorously solvable tight-binding single-band model – treating both the CPP-GMR and the exchange coupling $J$ on equal footing – and found that asymptotically both quantities share the same oscillation period (consistent with the Fermi surface topology) and have predominantly opposite phases. Since according to Ref. 19 the CPP-GMR is rather non-sensitive to impurities, our statements should also apply if additionally impurities are taken into account.

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20 In Ref. 13 we found additionally a Giant Magneto-Thermopower-Effect, which is also opposite in phase to GMR.
**Figure Captions**

Fig. 1: CPP-GMR of the systems \( n_f F/n_s S/n_f F \) (where \( n_f \) and \( n_s \) are the number of ferromagnetic and non-magnetic spacer monolayers, respectively). Majority spin electrons have the potentials \( V_{\uparrow} = -1.8 \) in the ferromagnets (all other potentials are 0), \( E_F = 2.5 \).

Fig. 2: Fermi ”surfaces” of the systems under consideration consist 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 \( V_{\uparrow} = -1.8 \)).

Fig. 3: GMR (solid line) and exchange coupling \( (J) \) (dashed line) vs. the spacer thickness, for \( n_f = 3, E_F = 2.5 \) and \( V_{\uparrow} = -1.8 \).

Fig. 4: The same as Fig. 3, but with \( n_f = 7 \) and for higher values of \( n_s \) to reveal the asymptotic trend of the oscillations.

Fig. 5: The same as Fig. 4, but with \( n_f = 5, E_F = 2.1 \), and \( V_{\uparrow} = -2 \).
Fig. 1:
Fig. 3:
Fig. 4:
Fig. 5: