Unusual beats of the perpendicular-current giant magneto-resistance and thermopower of magnetic trilayers

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(received July 1996)

Oscillations of the giant magneto-resistance (GMR) and thermo-electric power (TEP) vs. both the thickness of the non-magnetic spacer and also that of the ferromagnetic slabs are studied in the current-perpendicular-to-plane (CPP) geometry of magnetic trilayer systems, in terms of a single-band tight-binding model without impurities. The spin-dependent conductance has been calculated from the Kubo formula by means of a recursion Green’s function method and the semi-infinite ideal-lead wires trick. Additionally the TEP is obtained directly from Mott’s formula. In general, the thickness oscillations of the GMR and the TEP may have just one or two (short and long) oscillations. The long period, related to spectacular beats, is apparently of non-RKKY type. The TEP oscillations are strongly enhanced with respect to those of the GMR, have the same periods, but different phases and a negative bias.

The phenomenon of giant magnetoresistance (GMR) in magnetic multilayers has been intensively studied both experimentally\textsuperscript{[2]} and theoretically\textsuperscript{[3]} for more than five years now. After the paper\textsuperscript{[1]} was published it has become clear that one can expect a large magnetoresistance even in systems which have no impurities and no structural defects. As pointed out in\textsuperscript{[7]}, the GMR-oscillations have not only RKKY- type components, but may additionally reveal large particular non-RKKY oscillations (see below). For the case of semi-infinite ferromagnetic slabs, a period of those extra oscillations with the spacer thickness in the CPP (current-perpendicular-to-plane) geometry has been shown in\textsuperscript{[7]} to originate from values of the in-plane wavenumber $k_\parallel$ at which at least one spectral density vanishes at the ferromagnetic interface.

In the present letter we study the CPP-GMR (current-perpendicular-to-plane) behaviour of layered systems of the type $W/F_1/S/F_2/W$, where $W$ stands for a semi-infinite ideal lead wire, $F_1$ and $F_2$ for different ferromagnets, generally with different thicknesses, and $S$ for the non-magnetic spacer. Thus, apart from the leads, we are dealing with the usual magnetic trilayer systems. Our aim is to show that very pronounced beats may also, under some circumstances, appear as a function of the thicknesses of the ferromagnetic slabs. Besides the giant magneto-resistance effect, we also calculate the corresponding effect for the thermo-electric power (TEP).

The calculation technique, we have developed, is based on the Green’s function recursion method\textsuperscript{[6]}; it is close to that of\textsuperscript{[8]} with one essential exception, namely instead of working with finite systems in the in-plane space (x, y directions), we have reduced the whole problem to one dimension by performing the Fourier transform in the infinite x-y plane. Hence, our Green’s functions fulfill the following equation:

\begin{equation}
\sum_{z''} [(E_F - A_{zz''})\delta_{z,z''} - t_{zz''}] G_{\sigma}(k_{\|}, z'', z') = \delta_{z,z'}, \tag{1}
\end{equation}

where for the simple cubic lattice $t_{z,z'} = t \delta_{z', z\pm 1}$ and

\begin{equation}
A_{zz'} = V_\sigma(z) + 2t \cdot [\cos(k_z \cdot a) + \cos(k_y \cdot a)]. \tag{2}
\end{equation}

In eqn.(2), $E_F$ is the Fermi energy; $t$ ($< 0$) is the nearest-neighbour hopping integral; $a$ is the lattice constant, and $V_\sigma(z)$ is the spin-dependent atomic potential, which we assume to be constant for given material. Hereafter, both $|t|$ and the lattice constant are taken as energy- and length units, respectively, which formally corresponds to $t = -1$ and $a = 1$. The conductance of electrons of spin $\sigma$ is given by the well-known Kubo formula, which in turn may be expressed in terms of Green’s functions. In our case the relevant Green functions are defined by eqn. (1), and the conductance reads:

\begin{equation}
\Gamma_\sigma = \frac{8e^2 N_x N_y}{h(2\pi)^2} \int_{BZ} d^2k_{\|} [G''_\sigma(i, i)G''_\sigma(i - 1, i - 1) - G''_\sigma(i, i - 1)^2]. \tag{3}
\end{equation}

Here the index $i$, which counts the z-planes, is arbitrary, since the same amount of current flows through every cross-section. $G''$ stands for the imaginary part of $G$, and the integration is over the 2-dimensional Brillouin zone. We refer the reader to Refs.\textsuperscript{[2,3]} for the detailed description how the Green functions of interest can be found from recursion equations, and we only mention that due to the ideal-leads trick, the first step of the iteration is analogous to what is known as the square-root terminator in the continuous fractions method\textsuperscript{[9]}. The prefactor in Eq. (3) contains the conductance quantum $e^2/h$ as well as the cross-section area $N_x N_y$ to which the number of active conductivity channels is proportional.
Due to this effective reduction of the problem to one dimension, we could easily compute, by a rapid recursion procedure, the Greens functions in eq. (3) for a large number of $\vec{k}$-vectors and afterwards perform the integration of eqn. (3) very accurately by means of the highly efficient special $k$-points method of Cunningham [10]. The GMR has been defined as

$$GMR = \frac{\Gamma_{↑↑} + \Gamma_{↑↓}}{\Gamma_{↑↑} + \Gamma_{↑↓}} - 1,$$

(4)

where the superscripts of $\Gamma$ refer to the parallel and antiparallel magnetization configurations of the two ferromagnets, whereas the subscripts refer to the carriers considered.

Before we performed original calculations, we have tested our programs by considering systems studied by Asano et al. in [6], namely: (i) a non-magnetic multilayer $/A/B/A/B$ consisting of 4 sublayers, each three monolayers thick with alternating $\pm$ potentials, and (ii) their model for the FeCr superlattice: We have found very good agreement concerning both the CPP-GMR per unit area as well as the densities of states at the Fermi level, although the system of [6] has got only $12 \times 12$ atoms in the x-y plane and uses free boundary conditions.

Our results for the CPP-GMR of the $W/F_{1}/S/F_{2}/W$ systems are presented in the figures below. The plots correspond to the atomic potentials equal zero for both up- and down-spin electrons in the spacer and in the infinite lead wires. In the ferromagnets, the potentials for electrons with spin $\sigma = \pm 1$ take the following values: $V_{1\sigma}$ and $V_{2\sigma}$ for the $↑↑$-configuration and $V_{1\sigma}$ and $V_{2(-\sigma)}$ for the $↑↓$-configuration, where $V_{1\sigma}$ resp. $V_{2\sigma}$ and $V_{2(-\sigma)}$ concern the slabs $F_{1}$ and $F_{2}$, respectively. The actual values are given below and are also denoted in the figure captions. Additionally we have assumed a perfect matching of the minority bands of the ferromagnets with the spacer bands by putting $V_{1}\downarrow = V_{2}\downarrow = 0$ (cf. [8]). Finally, unless otherwise stated, we have chosen the Fermi energy $E_{F} = 2.5$ well above the potential barriers, see below.

It can be seen from Fig.1 and Fig.2 that the CPP-GMR oscillates as a function of the thickness $n_{f}$ of one or both ferromagnetic sandwiches with a short period of $\approx 2$ monolayers (ML). Additionally, in Fig.1, but not in Fig.2, pronounced beats are observed with typical repetition lengths of roughly 10 ML. Apparently those beats always appear, if the depth of the potential well corresponding to the ferromagnetic sandwich(es) with varying thickness is $V_{2\uparrow} = -1.8$ (Fig.1) or $-1$ (not shown), whereas in case of $V_{2\uparrow} = -2$ the beats are absent (Fig.2).

In case of Fig.3, where again $V_{2\uparrow} = -2$, but where only the spacer thickness $n_{s}$ is varied, one observes an intermediate period of $\approx 4.5$ ML, whereas the beats do not appear.

FIG.1: CPP-GMR of the system $3F_{1}/6S/n_{f}F_{2}$ between two infinite lead wires. $V_{1\uparrow} = -2$ and $V_{2\uparrow} = -1.8$ in the ferromagnets (all other potentials are 0). $E_{F} = 2.5$. Similar results apply for the system $n_{f}F_{1}/6S/n_{f}F_{1}$ with $V_{1\uparrow} = V_{2\uparrow} = -1.8$.

FIG.2: The same as Fig.1, but with $V_{1\uparrow} = V_{2\uparrow} = -2$. Again similar results apply for the system $n_{f}F_{1}/6S/n_{f}F_{1}$ with $V_{1\uparrow} = V_{2\uparrow} = -2$.

FIG.3: The same as Fig.2, but with $n_{f} = 3$ on both sides, as a function of the spacer thickness $n_{s}$.
In any case it can be easily seen that the GMR oscillations decay always roughly \( \sim n_f^{-1} \), analogously to the findings of Mathon et al. concerning the oscillations vs. the spacer thickness observed in [2]. It results from these observations that oscillations and beats of the GMR, similarly as those of the exchange coupling, see [2], are not specific for the non-magnetic spacer, but concern the ferromagnetic \( |B|_{\text{slabs}} \), too.

In the following we try to identify the RKKY- and non-RKKY periods visible in our figures, using arguments along the lines of [11].

In [11] Mathon et al. observed roughly analogous behaviour of the GMR as a function of the spacer thickness in a simpler system, namely a spacer imbedded between two identical semi-infinite ferromagnets. As in our case, the authors of [7] assume that within the spacer the potential \( V(z) \) vanishes, but concerning the ferromagnets their assumptions are different, since they assume the same vanishing potential for electrons with majority spin, but a positive potential \( V \) for electrons with minority spin, so that in their case the spacer represents a potential well for minority carriers. (In contrast, in our case we have a negative potential for majority-spin carriers in the ferromagnets, but vanishing potential for minority carriers, so that in our case the ferromagnets represent quantum wells for majority carriers, which are interrupted by a barrier represented by our spacer and bounded from outside by the ideal leads, which have the same potential as the spacer.) It was shown in [11] that (i) a continuum of wavenumbers \( k_z \) contributes to the conductivity \( \Gamma \), i.e. the dependence on the varying thickness \( L \) was \( \Gamma \sim \int \Delta k_x \Delta k_y \cdot c(k_x, k_y) \cdot \exp[2i(k_x k_y)] \) \( \Delta L \), and (ii) that dominating contributions can arise a) from wavenumbers, where \( k_z(k_x, k_y; E_f) \) is stationary as a function of \( (k_x, k_y) \), and b) from particular cut-off wavenumbers \( (k_z, k_y) \), where \( c(k_x, k_y) \) vanishes abruptly. These cut-off wavenumbers correspond in our case to unbound majority carriers which in \( z \)-direction have just the minimal kinetic energy in the wires to evade to infinity. The contributions under a) and b) are the "RKKY" and "non-RKKY-contributions" mentioned already above.

At this place one should note in any case that the "non-RKKY wavenumbers" under b) do not play a role in the thickness-dependence of the exchange coupling of the ferromagnets across the spacer, see [11].

In both cases a) and b), one can estimate the important wave numbers \( k_z \) from the asymptotic equation (valid actually for large thicknesses \( n_f \) and constant potential)

\[
k_z(k_x, k_y; E_f) = \arccos \left( \frac{V_o - E_f}{2} - \cos k_x - \cos k_y \right). \tag{5}
\]

Here, in case a), with \( V_o=2.5 \) and the values \( (k_x, k_y)=(\pm \pi, \pm \pi) \), where \( \cos k_x + \cos k_y \) is extremal, we get \( k_z^{(1)}=0.722 \) for the carriers with \( V_o = 0 \) (i.e. for the down-spin and spacer carriers in case of aligned ferromagnets), and \( k_z^{(2)}=1.721 \) for the up-spin carriers with \( V_o = -1.8 \) and \( k_z^{(2)} = 1.823 \) for \( V_o = -2 \). The corresponding wavelengths can then be calculated as in [11] from the expression:\n
\[
\lambda(p, q) = \pi/((pk_z^{(1)} + qk_z^{(2)})),
\]

which yields \( \lambda(0,1) = 1.825 \) \( (V_o = -1.8) \) and \( \lambda(1,0) = 1.723 \) \((V_o = -2)\), i.e. \( \sim \) the short period of two monolayers (2 ML) seen in the figures. It is interesting that in Fig.3, where only the spacer thickness is varied, only a longer wavelength of \( \sim 4.5 \) ML is visible, which would correspond to \( \lambda(1,0) = 4.35 \). However, these particular "RKKY-wavenumbers" would apparently not produce the beats in Fig.1, which have a much larger repetition length of \( \approx 10 \)ML.

In order to get the beats seen in Fig. 1 and in Fig.4 below, one needs apart from the wave characterized by \( k_z^{(2)} \) another wave with a wavenumber very close to it. As there seems no way to get such a wave from eqn. (5) with \( V_o = -1.8 \), we suggest it to be of non-RKKY character. This means, it should come from electrons at \( E = E_f \) with values of \( (k_x, k_y) \neq (\pm \pi, \pm \pi) \). More insight into the nature of non-RKKY oscillations can perhaps only be gained by taking into account localized and resonant states in addition to the extended ones used for the sketchy estimations of the RKKY wavenumbers above: In fact, although the localized states do not contribute directly to the conductance, they modify the density of states at \( E_f \) and thereby influence the conductivity.

In addition to the conductance \( \Gamma(E_f) \), where \( E_f \) is the Fermi energy, we also calculated the thermopower \( S \):

\[
S(\sigma) = -\frac{\pi^2 k_B T}{3|e|} (d/dE) \log \Gamma(\sigma) \tag{6}
\]

at \( E = E_f \), where \( \sigma \) denotes the spin of the carriers, \( T \) the Kelvin temperature, \( k_B \) Boltzmann’s constant and \( e \) the elementary charge.

Analogously to the GMR, see eqn. [4], we define the "Giant Magneto-TEP-effect" \( GMTEP \), where \( TEP \) means thermo-electric power, by...
\[ GMTEP = \frac{S_{\uparrow \uparrow} + S_{\downarrow \downarrow}}{S_{\uparrow \downarrow} + S_{\downarrow \uparrow}} - 1. \]  

(7)

It can be seen in Fig.4 that the oscillations of the GMTEP are even stronger than those of the GMR, although they have a significant and negative bias and a different phase than those of the GMR.

Finally it should be noted that the amplitude of the oscillations observed in the figures 1 and 2 is typically of the order of 1% to 2% only: Thus the oscillations can only be detected by very accurate calculations as the present one, and only with interfaces of sufficient quality: In fact, we have ”smeared” the results for GMR(i) as follows

\[ GMR(i) \rightarrow (x/2) \cdot [GMR(i+1) + GMR(i-1)] + (1-x) \cdot GMR(i), \]  

(8)

with \( x = 0.5 \) and \( x = 0.25 \), respectively, and obtained instead of Fig.1 the ”smeared” Fig.5, where the oscillations are no longer visible for strong interdiffusion \( (x = 0.5) \), whereas for \( x = 0.25 \), they are roughly reduced by a factor \((1/2)\) and can still be recognized.

\[ 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35 \quad 40 \quad 45 \quad 50 \]

\[ 1.6 \quad 1.64 \quad 1.68 \quad 1.72 \]

GMR

FIG.5: The same as Fig.1, but smeared in accordance with eqn. (8) with \( x = 0.25 \) (dashed line) and \( x = 0.5 \) (solid line).

In conclusion, within an s-band tight-binding model combined with the Green’s function recursion method, we have reduced the calculation of the CPP-GMR effectively to one dimension. We have computed the CPP-GMR for pure systems composed of two different ferromagnets separated by a non-magnetic spacer and sandwiched between ideal infinite lead wires. Unusual beats of the GMR vs. the thickness of the ferromagnetic slabs have been observed and shown to depend strongly on the kind of ferromagnetic slabs (i.e. on the potentials \( V_{\sigma} \) representing the exchange splittings). Similar results, with even stronger beats, have also been obtained for the ”Giant Magneto-TEP-Effect”, where ”TEP” means the Thermo-Electric Power. The beats of the GMR have been shown to remain visible, if there is only moderate chemical interdiffusion in the boundary layers. Finally, it has been shown that the short periods of 2 monolayers visible in the results arise from the usual ”RKKY”-type mechanism, whereas the beats arise from certain ”non-RKKY” cut-off contributions, analogous to those suggested in [7].

Acknowledgements

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

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