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Selection rules for oscillations of the giant magnetoresistance with nonmagnetic spacer layer thickness

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Oscillations of the giant magnetoresistance (GMR) with nonmagnetic spacer layer thickness are predicted in the current-perpendicular-to-plane (CPP) geometry. The methods of the quantum-well theory of the oscillatory exchange coupling are applied to the Kubo formula to derive general selection rules for the GMR oscillation periods. The selection rules are illustrated for single-orbital tight-binding and parabolic band models. They predict that the CPP GMR oscillates not only with the expected Fermi-surface period but also with additional periods determined by the potential steps between the magnetic and nonmagnetic layers.

Since the discovery of the giant magnetoresistance effect (GMR) (Ref. 1) and oscillatory exchange coupling[2] the transport and magnetic properties of magnetic multilayers have attracted much attention. To explain the oscillations in the exchange coupling, Edwards and Mathon[3,4] have proposed that spin-dependent potentials in the ferromagnetic layers create quantum-well states in the nonmagnetic spacer layer sandwiched between the magnetic layers. As the thickness of the spacer is varied, the passage of quantum-well states across the Fermi surface (FS) causes oscillations in the exchange coupling, the oscillation periods being determined by the spacer FS.[4] The oscillatory exchange coupling is, therefore, inherently a quantum interference effect.

On the other hand, the conventional explanation[5] of the GMR effect is based on spin-dependent scattering of electrons from magnetic impurities at the magnet/spacer interfaces. The spin-dependent scattering is usually treated within the classical Boltzmann equation formalism[5] and the scattering of electrons from quantum wells in the magnetic multilayers is considered to be unimportant. This conventional point of view was challenged recently by Schep *et al.*[6] who showed that, at least in the current-perpendicular-to-plane (CPP) geometry, a very large GMR can be obtained without any impurity scattering. They applied the Landauer-Buttiker scattering formalism[7] to ballistic point contacts of Co/Cu multilayers and found a CPP GMR of more than 120%. The whole GMR effect in this regime is due to reflections of electrons from quantum wells/barriers and, therefore, has the same origin as the oscillatory exchange coupling.

The purpose of this contribution is to show that the GMR mechanism proposed by Schep *et al.*[6] leads necessarily to oscillations of the CPP GMR with the spacer thickness. Applying the methods of the quantum-well theory of the oscillatory exchange coupling[4] to the Kubo formula for the conductivity,[8] we derive general selection rules for the periods of oscillations of the GMR. The selection rules are illustrated for parabolic and single-orbital tight-binding bands. The most surprising result we obtain is that the GMR in the CPP geometry oscillates not only with the FS oscillation period obtained for the exchange coupling[4] but there are additional periods determined by the heights of the potential steps between the magnetic and nonmagnetic layers. This is in contrast to the results of Vedyaev *et al.*[9] who obtained quantum oscillations of GMR in the current-in-plane (CIP) geometry but only with the FS period.

We consider a trilayer consisting of two magnetic layers of M atomic planes each separated by a nonmagnetic spacer layer of N atomic planes. The trilayer is sandwiched between two semi-infinite ideal lead wires.[8] Both the trilayer and lead wires are described by a simple cubic single-orbital tight-binding Hamiltonian with nearest-neighbor hopping t. We take (001) orientation of the layers and measure all the energies in units of t. Following Schep *et al.*,[6] we assume perfect interfaces and neglect the effect of impurities. It follows that the wave vector $\mathbf{k}_{\parallel}$ parallel to the layers remains a good quantum number. The conductance Γ of the trilayer in its ferromagnetic (FM) or antiferromagnetic (AF) configuration is the sum of the conductances of the up- and down-spin electrons. The CPP GMR is defined by[6] $GMR=(\Gamma_{\rm FM}^{\uparrow}+\Gamma_{\rm FM}^{\downarrow}-2\Gamma_{\rm AF}^{\uparrow,\downarrow})/2\Gamma_{\rm AF}^{\uparrow,\downarrow}$. For any particular configuration, the CPP conductance of electrons of spin σ is given by the Kubo formula[8]

$$\Gamma^{\sigma}=(2e^2/h)\sum_{\mathbf{k}_{\parallel}}[\tilde{G}_{00}^{\sigma}\tilde{G}_{11}^{\sigma}+\tilde{G}_{11}^{\sigma}\tilde{G}_{00}^{\sigma}-\tilde{G}_{01}^{\sigma}\tilde{G}_{01}^{\sigma}-\tilde{G}_{10}^{\sigma}\tilde{G}_{10}^{\sigma}], \quad (1)$$

where $\tilde{G}=(1/2i)[G^{-}-G^{+}]$, G^{-}, G^{+} are the advanced and retarded Green's functions evaluated at the Fermi energy E_F, the indices 0, 1 label any two neighboring atomic planes in the spacer, and the trace is over all $\mathbf{k}_{\parallel}$ in the two-dimensional Brillouin zone. The Green's functions are calculated assuming that the electrons are noninteracting in the spacer and experience exchange-split one-electron potentials in the ferromagnets. It is straightforward to generalize Eq. (1) for the conductance to an arbitrary tight-binding Hamiltonian. However, we restrict our discussion here to a single-orbital band because one can derive closed expressions for all the Green's functions in Eq. (1) and oscillations of the conductance can be discussed without resort to numerical calculations.

To calculate the required matrix elements of G we pass an imaginary cleavage plane between the atomic planes 0 and 1, which separates our infinite sample into two independent semi-infinite systems. We refer to them as the left and right overlayers on the ideal leads. It is easy to show using

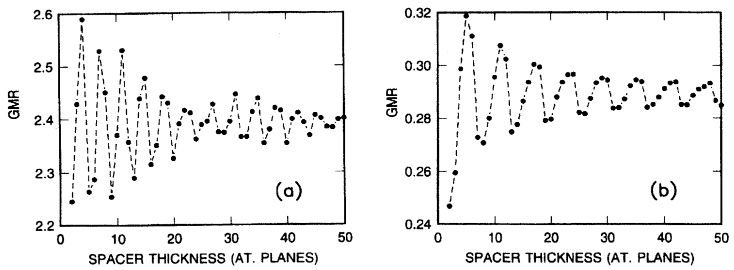

FIG. 1. Dependence of the CPP GMR on the nonmagnetic spacer layer thickness. Tight-binding model: (a) $E_F=0.8,\Delta=0.6$; (b) $E_F=0.8,\Delta=0.3$.

Dyson's equation that $G_{00}=(1-g_{00}g_{11})^{-1}g_{00}$, $G_{11}=(1-g_{00}g_{11})^{-1}g_{11}$, and $G_{01}=G_{10}=g_{00}G_{11}$, where g_{00} and g_{11} are the surface matrix elements of the Green's functions for the isolated left and right overlayers. We shall further require the matrix elements of the tight-binding Green's function g_{mn}^{sl} of an isolated (001) slab of i atomic planes. They can be obtained by inverting algebraically the $i\times i$ matrix $(IE-H)$, where H is the slab Hamiltonian and I is a unit matrix

$$g_{mn}^{sl}=\frac{(-1)^{m-n+1}\sin(mk_\perp a)\sin(n-i-1)k_\perp a}{\sin(k_\perp a)\sin(i+1)k_\perp a}. \quad (2)$$

Here a is the lattice constant, $m\leqslant n=1,2,\ldots,i$, and $k_\perp(E=E_F,\mathbf{k}_\|)$ is the wave vector normal to the layers at the bulk spacer FS.

Suppose that there are i atomic planes of the spacer contained in the left overlayer. We determine analytically the left overlayer Green's function g_{00}^σ by "grafting" an isolated slab of i atomic planes of the spacer on the left ferromagnet. This is achieved by restoring hopping between the slab and ferromagnet via the Dyson equation. Assuming that the surface Green's function for the left g_L ferromagnet is known, it is easy to show that g_{00} is given by

$$g_{00}^\sigma=g_{ii}^{sl}+g_{i1}^{sl}(1-g_L^\sigma g_{ii}^{sl})^{-1}g_L^\sigma g_{1i}^{sl}. \quad (3)$$

Similarly, we obtain g_{11}^σ for the right overlayer. Substituting now from Eqs. (2) and (3) in Eq. (1), we arrive at a remarkably simple expression for the conductance in terms of g_L and g_R:

$$\Gamma^\sigma=\sum_{\mathbf{k}_\|}\Gamma^\sigma(\mathbf{k}_\|)=\sum_{\mathbf{k}_\|}\frac{4e^2\sin^2(k_\perp a)\mathrm{Im}g_L^\sigma\mathrm{Im}g_R^\sigma}{h|\sin(N+1)k_\perp a-(g_L^\sigma+g_R^\sigma)\sin(Nk_\perp a)+g_L^\sigma g_R^\sigma\sin(N-1)k_\perp a|^2}. \quad (4)$$

In fact, the partial conductance $\Gamma^\sigma(\mathbf{k}_\|)$ in Eq. (4) is the transmission coefficient[7,8] of electrons having an energy $E=E_F$ and parallel wave vector $\mathbf{k}_\|$. The key feature of $\Gamma^\sigma(\mathbf{k}_\|)$, seen explicitly in Eq. (4), is that its dependence on the spacer thickness $L=Na$ is periodic. We thus expect that the total conductance in each spin channel, and the GMR itself, should also oscillate as a function of L. To clarify the physics involved, we first discuss oscillations of the conductance in the simplest case of a spacer sandwiched between two semi-infinite ferromagnets. It follows that electrons are scattered from a single potential well or barrier having a different height for the up- and down-spin carriers. To model qualitatively the situation in Co/Cu (Ref. 6) or Fe/Cr, we assume perfect matching of bands between the ferromagnet and spacer in the up-spin (majority) channel. There is, therefore, a potential well for down-spin (minority) holes in the spacer layer but no wells or barriers for the majority carriers.

It is straightforward to compute the GMR from Eq. (4) but, as in the case of oscillatory exchange coupling,[4] a very large number of $\mathbf{k}_\|$ points is required to achieve convergence. Typically, we use about 8000 $\mathbf{k}_\|$ points in the irreducible segment of the two-dimensional Brillouin zone. The computed GMR is shown in Fig. 1 for two qualitatively different situations. In the first case [Fig. 1(a)], the Fermi energy $E_F=0.8$ and the exchange splitting $\Delta=0.6$ in the ferromagnet (measured in units of the hopping) were chosen so that E_F lies close to the top of the spacer potential well in the down-spin channel. In the second case [Fig. 1(b)], E_F lies some distance above the top of the well $(E_F=0.8,\Delta=0.3)$. In both cases, well-defined oscillations of GMR with spacer thickness L occur. In contrast to the exchange coupling, the CPP GMR oscillations have a large constant bias equal to the asymptotic value of the GMR reached for large L.

The most remarkable feature seen in Fig. 1(a) are beats which clearly demonstrate the presence of two periods in the case when E_F lies close to the top of the well. We recall that the exchange coupling evaluated for the same model[3,4] oscillates with a single period determined by the Fermi wave vector in the spacer layer. Moreover, the single period seen in Fig. 1(b) is not the FS period obtained for the exchange coupling. The presence of additional periods indicates that a qualitatively different mechanism is involved in the CPP GMR, and we now proceed to identify it. To explain the origin of the oscillation periods of the GMR, we exploit the fact that the transmission coefficient $\Gamma^\sigma(\mathbf{k}_\|)$ is periodic in L. The conductance given by Eq. (4) can, therefore, be expanded in a Fourier series

$$\Gamma^\sigma=\mathrm{Re}\sum_{\mathbf{k}_\|}\sum_r c_r^\sigma(\mathbf{k}_\|)e^{2irNk_\perp(\mathbf{k}_\|)a}, \quad (5)$$

where c_r^σ is the Fourier coefficient of $\Gamma^\sigma(\mathbf{k}_\parallel)$ and $k_\perp$ is defined in Eq. (2). The Fourier series representation (5) enables us to separate the oscillatory part of the GMR ($r\neq 0$) from the nonoscillatory background ($r=0$). Applying asymptotic expansions[4] valid for large spacer thickness L to the oscillatory component, we can derive general selection rules for the oscillation periods.

For large L, the imaginary exponential in Eq. (5) oscillates rapidly as a function of $\mathbf{k}_\parallel$ and, therefore, the contributions to the sum in Eq. (5) from different $\mathbf{k}_\parallel$ tend to cancel. There are only two situations in which the cancellation does not occur: (a) in the vicinity of a point $\mathbf{k}_\parallel^0$ at which the phase $k_\perp(E_F,\mathbf{k}_\parallel)$ is stationary; (b) in the vicinity of a boundary at which the sum over $\mathbf{k}_\parallel$ terminates abruptly. It follows that we first need to identify all the stationary points $\mathbf{k}_\parallel^0$ of $k_\perp(E_F,\mathbf{k}_\parallel)$ and all the cutoff points $\mathbf{k}_\parallel^{cp}$ at which $\Gamma(\mathbf{k}_\parallel)$ vanishes. All possible oscillation periods of the conductance (GMR) are then given by $\pi/k_\perp(E_F,\mathbf{k}_\parallel^0)$ and $\pi/k_\perp(E_F,\mathbf{k}_\parallel^{cp})$.

Case (a) requires no special discussion since the periods coming from the stationary points of $k_\perp(E_F,\mathbf{k}_\parallel)$ are exactly the same as the periods of the oscillatory exchange coupling.[4] Case (b), however, is new and has no analog in the theory of oscillatory exchange coupling. To guide us in the formulation of general selection rules, we first analyze a trilayer with two semi-infinite ferromagnets. It follows from Eq. (4) that the boundary in $\mathbf{k}_\parallel$ space at which $\Gamma(\mathbf{k}_\parallel)$ vanishes is defined by

$$\mathrm{Im}g_L^\sigma=0 \quad \text{and/or} \quad \mathrm{Im}g_R^\sigma=0, \tag{6}$$

where "or" applies in the AF configuration. The selection rule (6) has a simple physical interpretation. In the CPP geometry the conductance in a channel $\mathbf{k}_\parallel$ vanishes when the electrons at E_F with that particular value of $\mathbf{k}_\parallel$ become totally reflected from either the left or right ferromagnet. That happens when the state $(E_F,\mathbf{k}_\parallel)$ lies outside the band of the left (right) ferromagnet, in which case the corresponding spectral density $\mathrm{Im}g_L^\sigma(\mathrm{Im}g_R^\sigma)$ vanishes.

The selection rules for the oscillation periods of the conductance are necessary but not sufficient conditions. Whether any particular oscillation with a period predicted by the selection rules is actually seen depends on its amplitude. The amplitude and its decay with the spacer thickness L can be determined from asymptotic expansions of the conductance valid for large L. We first derive general asymptotic expansions for oscillations originating from the stationary points.

Consider a point (k_x^0,k_y^0) in the $\mathbf{k}_\parallel$ plane at which $k_\perp$ is stationary. Following Ref. 4, we expand $k_\perp(E_F,\mathbf{k}_\parallel)$ in the argument of the exponential in Eq. (5) up to second order in k_x,k_y about (k_x^0,k_y^0) and convert the sum over k_x,k_y into an integral. For large L, rapid oscillations of the imaginary exponential in Eq. (5) ensure that only a small neighborhood of (k_x^0,k_y^0) contributes to the integral. The Fourier coefficient in Eq. (5) can, therefore, be approximated by its value at (k_x^0,k_y^0). The remaining integrals with respect to k_x,k_y are Gaussian and can be readily evaluated. This leads to the following oscillatory contribution to the conductance in a spin channel σ at the stationary point (k_x^0,k_y^0):

$$\Gamma_{\mathrm{FS}}^\sigma=(N_\parallel/4\pi)\mathrm{Re}\sum_{r=1}^{\infty}\tau c_r(\mathbf{k}_\parallel^0)m^*\,e^{2irk_\perp^0 aN}/rN. \tag{7}$$

Here, $m^*=|[\partial^2(k_\perp a)/\partial(k_x a)^2][\partial^2(k_\perp a)/\partial(k_y a)^2]|^{-1/2}$ is the curvature of the FS at the stationary point and $\tau=i$ when both derivatives in m^* are positive, $\tau=-i$ when they are negative, and $\tau=1$ when the two derivatives have opposite signs. It can be seen that the conductance oscillates with period $\pi/k_\perp^{\mathrm{FS}}$, where $k_\perp^{\mathrm{FS}}$ is the extremal radius of the spacer FS in the direction perpendicular to the layers. The oscillation amplitude decreases asymptotically as $1/L$ and its overall magnitude is controlled by two factors: the curvature of the spacer FS and the value of the Fourier component of the transmission coefficient at the stationary point. The latter depends on matching of the bands in the direction normal to the layers along the line $\mathbf{k}_\parallel=(k_x^0,k_y^0)$. As discussed elsewhere[10] in the context of the oscillatory exchange coupling, an asymptotic expansion of the type (7) is valid for an arbitrary tight-binding band structure.

An asymptotic expansion about a cutoff point of the transmission coefficient is more difficult and we describe it here only for a parabolic band model of a trilayer with semi-infinite ferromagnets and perfect band match in the up-spin channel. It follows that only the asymptotic expansion of the oscillatory conductance in the down-spin channel is required. The conductance is the sum over all $\mathbf{k}_\parallel$ of the transmission coefficient[11] for a quasi-one-dimensional potential well of width L and depth V. Converting the sum over $\mathbf{k}_\parallel$ to an integral over the parallel energy $E_\parallel=\hbar^2k_\parallel^2/2m$, we find that the conductance Γ normalized to the conductance of an ideal spacer (without a potential well) is given by

$$\Gamma=(1/E_F)\times\int_{0\leq E_\parallel\leq E_F-V}\left[1+\frac{V^2\sin^2(k_\perp L)}{4(E_F-E_\parallel)(E_F-E_\parallel-V)}\right]^{-1}dE_\parallel, \tag{8}$$

where $k_\perp=(2m/\hbar^2)^{1/2}(E_F-E_\parallel)^{1/2}$ is the perpendicular wave vector at the spacer FS. The cutoff at the top of the well occurs at the upper limit $E_\parallel=E_F-V$ of the integral in Eq. (8). The integrand (transmission coefficient) in Eq. (8) is periodic in L with period $\pi/k_\perp$ and we expand it in a Fourier series. All the Fourier coefficients c_r are obtained analytically but, for simplicity, we keep only the fundamental oscillation $r=1$. After a substitution in Eq. (8) that makes the energy dimensionless, the Fourier expansion takes the form

$$\Gamma=\int_0^{E_F/V-1}c_1(u)\cos(2Lk_\perp^{cp}\sqrt{u+1})du, \tag{9}$$

where $k_\perp^{cp}=(2mV/\hbar^2)^{1/2}$ and the Fourier component c_1 is given by $c_1(u)=16(V/E_F)u(u+1)[1-(1-f^2(u))^{-1/2}]$ with $f(u)=[8u(u+1)+1]^{-1}$. It is now the lower limit $u=0$ which gives the cutoff at the top of the well. The upper limit $u=E_F/V-1$ leads to the FS oscillation with period $\pi/k_\perp^{\mathrm{FS}}$ and the corresponding asymptotic behavior of Γ is given by Eq. (7).

We now focus on the asymptotic expansion about the cutoff point at $u=0$. The expansion is nonstandard because $c_1(u)$ is not analytic at $u=0$. We first make the substitution

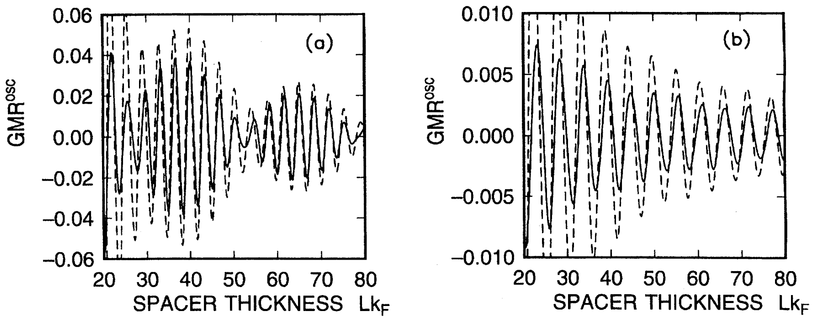

FIG. 2. Comparison of the oscillatory component of CPP GMR calculated from the asymptotic expansions (7) and (11) (dashed curves) with the exact results (solid curves) obtained by numerical integration of Eq. (9). Parabolic-band model: (a) $E_F/V=1.3$; (b) $E_F/V=3.0$.

$u+1=(x+1)^2$ in Eq. (9) and examine the leading term of $c_1(x)$ for $x\rightarrow 0$. It is easy to show that $c_1(x)\approx -4(V/E_F)(2x)^{1/2}$. Approximating $c_1(x)$ by this leading term over the whole integration range and integrating by parts in Eq. (9), we obtain

$$\Gamma_{cp}=(2\sqrt{2}V/E_F k_\perp^{cp} L)\int_0^\infty \frac{\sin[2k_\perp^{cp}L(x+1)]}{\sqrt{x}}dx, \quad (10)$$

where we have extended the upper limit of integration to ∞. This is justified since the contribution to the asymptotic expansion from $x\rightarrow\infty$ vanishes and the correct asymptotic contribution from the upper limit $E_F/V-1$ has already been isolated in Eq. (7). The fact that we are approximating the integrand by the leading term for small x everywhere is immaterial since contributions from all x other than $x\approx 0$ cancel. The integral in Eq. (10) is standard and the asymptotic expansion Γ_{cp} takes the form

$$\Gamma_{cp}=2\sqrt{\pi}(V/E_F)\frac{\sin(2k_\perp^{cp}L+\pi/4)}{(k_\perp^{cp}L)^{3/2}}+O[(1/k_\perp^{cp}L)^2]. \quad (11)$$

It follows that the period $\pi/k_\perp^{cp}$ is determined by the depth V of the spacer potential well. The oscillatory component of the GMR calculated from Eqs. (7) and (11) is compared in Fig. 2 with the exact results obtained by numerical integration of Eq. (9). The only parameter in Eq. (9) is the ratio E_F/V in the minority spin channel. The results in Fig. 2(a) are for E_F close to the top of the well ($E_F/V=1.3$) and those in Fig. 2(b) correspond to the opposite limit ($E_F/V=3.0$). The beats in Fig. 2(a) are well reproduced by the asymptotic formulas, which confirms that one of the periods comes from the FS and the other from the top of the well. The amplitude of the FS oscillation given by Eq. (7) is small for $E_F=3.0$ and, therefore, only the oscillation with the top-of-the-well period is seen in Fig. 2(b). It is interesting that both the parabolic and single-orbital tight-binding band models predict that the new top-of-the-well period is more robust than the FS period which is suppressed when the Fermi level lies well above the top of the well.

All our conclusions for semi-infinite ferromagnets remain valid qualitatively for magnetic layers of finite thickness. In this case, one has transmission across a double-barrier structure. There is now no complete cutoff at the top of the barrier modeling each ferromagnet since $\Gamma(\mathbf{k}_\parallel)=1$ for resonances inside the well. However, there is a finite number of such resonances in the well and their widths tend to zero rapidly as they move deeper in the well. It follows that one is integrating in Eq. (4) (Ref. 8) essentially a function which is nonzero only on a set of measure zero. There is, therefore, again an effective cutoff near the top of the well. Numerical integration of Eq. (4) confirms this conclusion.

Transmission resonances on ferromagnetic layers of finite thickness lead also to oscillations of the CPP GMR with the ferromagnet thickness. This effect, implicit in Eq. (4), will be discussed elsewhere. Oscillations of GMR with ferromagnet thickness have been observed by Okuno and Inomata[12] for Fe/Cr, but in the CIP geometry where we would expect this effect to be less pronounced.

Finally, it is important to clarify why the top-of-the-well period does not appear in the exchange coupling. The coupling is a total energy effect and, therefore, bound states inside the well contribute to it (but not to the conductance). The oscillatory contributions to the coupling from states just below and just above the top of the well cancel exactly since there is no discontinuity at the top of the well.[13] There is, therefore, no cutoff at the top of the well for the coupling and it oscillates only with the FS periods.

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