

Quantum oscillations of the spin density in magnetic multilayers

J. Mathon, A. Umerski, and Murielle Villeret

Department of Mathematics, City University, London EC1V 0HB, United Kingdom

R. B. Muniz

Departamento de Física, Universidade Federal Fluminense, Niteroi, Brazil

(Received 17 July 1998; revised manuscript received 12 October 1998)

An asymptotic stationary phase formula is derived for the oscillatory spin density induced in a nonmagnetic spacer sandwiched between two semi-infinite ferromagnets. It gives an explicit dependence for the polarization on the spacer layer thickness and on the distance from the ferromagnet-spacer interface. Both dependences are shown to oscillate with the same periods as the exchange coupling between the ferromagnetic layers. The magnitude of the polarization is governed by the degree of confinement of carriers in the spacer quantum well and by the curvature of the spacer Fermi surface. The formula is applied to a Co/Cu/Co (001) trilayer described by tight-binding bands fitted to an *ab initio* band structure. Its validity is tested against a fully numerical calculation using the same band structure. As in the case of the oscillatory exchange coupling, the induced polarization is dominated by the contribution of the Cu Fermi surface neck extrema leading to a short period oscillation of 2.6 atomic planes. An interesting non-Ruderman-Kittel-Kasuya-Yosida initial decay of the induced polarization is discussed. [S0163-1829(99)06309-2]

Oscillatory exchange coupling between two ferromagnetic layers separated by a nonmagnetic metallic spacer layer¹ is one of the rare manifestations of quantum interference effects in a metallic system structured on a nanometer length scale. It was proposed early on by Edwards and co-workers^{2,3} that the oscillatory exchange coupling is due to size quantization of the energy of electrons confined in a quantum well by the spin-dependent potentials of the magnetic layers. For large spacer layer thicknesses (≈ 10 atomic planes), an analytic formula for the coupling has been derived.²⁻⁴ The asymptotic formula is based on the stationary phase approximation and is referred to as analytic quantum well (AQW) formula. It allows us to determine the oscillation periods, amplitudes and rate of decay of the coupling unambiguously and relate them to the details of the band structures of the ferromagnets and nonmagnetic spacer. Applications of the AQW theory²⁻⁴ using a realistic band structure⁵⁻⁷ lead to oscillation periods and amplitudes of the coupling that are in agreement with numerical total energy calculations^{6,8-12} and also with experimental results for multilayers with noble metal spacers.¹³ The photoemission experiments of Ortega and Himpsel^{14,15} and Segovia *et al.*¹⁶ confirm the energy quantization of electrons confined in a nonmagnetic spacer layer.

Although it is assumed implicitly that quantum confinement of electrons leads also to oscillations of the spin density in the spacer layer, the spin density has never been analyzed analytically. The induced moment in a nonmagnetic spacer has been calculated numerically.¹⁷⁻¹⁹ A very small moment induced in Cu at the Co/Cu interface was previously detected by Samant *et al.*¹⁷ and Pizzini *et al.*²⁰ using circular dichroism and by Jin *et al.*²¹ using NMR. However, as in the case of oscillatory exchange coupling, such numerical calculations are computationally very demanding and do not allow explicit separation of oscillatory components arising from different extremal portions of the spacer Fermi surface (FS).

The purpose of this paper is to apply the stationary phase method of the AQW theory⁶ to calculate analytically the spin density in a nonmagnetic spacer layer sandwiched between two ferromagnets (trilayer). We demonstrate that the periods of oscillations of the induced moment are determined by the extremal radii of the bulk spacer Fermi surface. The amplitudes and asymptotic decay of oscillations depend on the curvature and the velocity of carriers at the Fermi surface extremal points, and on the matching between the ferromagnet and spacer bands. We apply the formula to Co/Cu/Co(001) trilayer and analyze the periods and amplitudes of the contributions arising from the different extrema of the Cu Fermi surface.

We consider a trilayer consisting of two semi-infinite ferromagnets separated by a nonmagnetic spacer layer of N atomic planes. The magnetizations of the magnetic layers are assumed to be either parallel or antiparallel and the spin quantization axis is chosen in the direction of the z axis. It is convenient to work in a mixed representation which is Bloch-like in the direction parallel to the planes of the trilayer and atomiclike in the perpendicular direction. Electronic states are, therefore, labeled by the plane index $R = 1, \dots, N$, wave vector \vec{k}_{\parallel} parallel to the layers, orbital index μ (for transition/noble metals, $\mu = 1, \dots, 9$), and the spin index σ . We describe the electronic structure of the trilayer using a tight-binding parametrization of an *ab initio* band structure. However, it will be seen that the implementation of the stationary phase theory relies only on the periodicity (quasiperiodicity) of the one-electron Green's function. This property is common to the tight-binding method we use, LMTO tight-binding,⁸ and layer KKR methods¹⁰ since they are all formulated in terms of local one-electron Green's functions. It is, therefore, immaterial which one of these methods one chooses as long as the one-electron energies of the trilayer are correctly reproduced. We stress, however, that the AQW formalism for the induced moment is not valid

for small spacer thicknesses and close to the ferromagnet/spacer interfaces, where a full numerical *ab initio* calculation is required. As in the case of oscillatory exchange coupling, electron-electron interactions are neglected in the spacer and the method is, therefore, not applicable to highly polarizable spacers such as Pd.

At zero temperature, the total spin polarization per atom $P(R, N)$ in an atomic plane R induced in a spacer of N atomic planes is given by

$$P(R, N) = -\frac{\hbar}{2\pi N_{\parallel}} \text{Im Tr} \sum_{\vec{k}_{\parallel}} \int_{-\infty}^{E_F} [\mathbf{G}^{\uparrow}(R, N, E, \vec{k}_{\parallel}) - \mathbf{G}^{\downarrow}(R, N, E, \vec{k}_{\parallel})] dE, \quad (1)$$

where $\mathbf{G}^{\sigma}(R, N, E, \vec{k}_{\parallel})$ is the diagonal matrix element (in the plane index R) of the one-electron Green's function, N_{\parallel} is the number of atoms in any atomic plane parallel to the trilayer, E_F is the Fermi energy, the trace is over all atomic orbitals, and the sum is over the two-dimensional Brillouin zone. It should be noted that $\mathbf{G}^{\sigma}(R, N, E, \vec{k}_{\parallel})$ is a matrix whose size is determined by the number of orbitals employed in the tight-binding parametrization (we use the convention that all the matrices are denoted by bold letters).

To calculate the local one-electron Green's function in an atomic plane R , it is convenient⁶ to separate the trilayer into two independent overlayers of R atomic planes on the left ferromagnet and $N-R$ atomic planes on the right ferromagnet. This is achieved by turning off electron hopping between the atomic planes R and $R+1$. We then proceed as follows. The surface Green's functions of the left and right semi-infinite ferromagnets are first determined by the analytical method of Umerski²² and then the left and right overlayers of the spacer material are deposited plane by plane using the method of adlayers⁶ or that of Ref. 22. After each deposition, the surface Green's function is updated from the Dyson equation. Finally, the trilayer is reconnected by switching on the electron hopping matrix $t(\vec{k}_{\parallel})$ between the planes R and $R+1$. The exact Green's function $\mathbf{G}^{\sigma}(R, N)$ in the plane R is obtained from the Dyson equation

$$[\mathbf{G}^{\sigma}(R, N)]^{-1} = [\mathbf{g}_{\leftarrow}^{\sigma}(R)]^{-1} - t^{\dagger}(\vec{k}_{\parallel}) \mathbf{g}_r^{\sigma}(N-R) t(\vec{k}_{\parallel}), \quad (2)$$

where we use the convention that capital letters denote Green's functions of the connected system and lower-case letters those of the cleaved system (the explicit dependence on E and \vec{k}_{\parallel} has been suppressed). In particular, $\mathbf{g}_{\leftarrow}^{\sigma}(R)$ is the surface Green's function of the left overlayer and $\mathbf{g}_r^{\sigma}(N-R)$ that of the right overlayer. It should be noted that Eq. (2) applies both to the ferromagnetic and antiferromagnetic configurations of the magnetic layers but, in the latter case, $\mathbf{g}_r^{\sigma}(N-R)$ needs to be replaced by $\mathbf{g}_r^{-\sigma}(N-R)$.

Equations (1) and (2) can be used to determine the local spin moment numerically, and the numerical results for Co/Cu(001) trilayer will be discussed later. However, Eqs. (1) and (2) are also the starting point for calculating the local moment analytically using the stationary phase method. Application of the stationary phase method is based on the observation that the surface Green's function (spectral density) $\mathbf{g}_{\leftarrow}^{\sigma}(R)$ of an overlayer of R atomic planes of the spacer material on a semi-infinite substrate is a periodic or quasiperi-

odic function of the overlayer thickness R . This result is proved rigorously in Ref. 22. For simplicity, we restrict ourselves in this paper to the case of an overlayer in which there is only one band intersecting the Fermi surface for each \vec{k}_{\parallel} . This is satisfied for the Cu (001) spacer. In this case, the surface Green's function is strictly periodic.²² Since this applies to the left and right independent overlayers, $\mathbf{g}_{\leftarrow}^{\sigma}(R)$ is periodic in the variable R and $\mathbf{g}_r^{\sigma}(N-R)$ in the variable $N-R$, both functions having the same period π/k_{\perp} , where k_{\perp} is obtained by solving the bulk spacer dispersion $E(k_{\perp}, \vec{k}_{\parallel}) = E_F$. It follows from Eq. (2) that the Green's function \mathbf{G}^{σ} of the connected trilayer can be regarded as a periodic function of two independent variables R and $S=N-R$.

Introducing $\rho = (-1/\pi) \text{Tr}[\mathbf{G}^{\uparrow} - \mathbf{G}^{\downarrow}]$, we can write the spin polarization in an atomic plane R of the spacer in the form

$$P(R, S) = \frac{\hbar}{2N_{\parallel}} \text{Im} \sum_{\vec{k}_{\parallel}} \int_{-\infty}^{E_F} \rho(R, S, E, \vec{k}_{\parallel}) dE. \quad (3)$$

Since ρ is a periodic function of two variables, it can be expanded in a double Fourier series in R and S . Writing the Fourier coefficients in complex form $c_{n,m}(E, \vec{k}_{\parallel}) = |c_{n,m}(E, \vec{k}_{\parallel})| \exp[i\psi_{n,m}(E, \vec{k}_{\parallel})]$, we obtain

$$\rho = \sum_{n,m} |c_{n,m}(E, \vec{k}_{\parallel})| e^{i[\phi_{n,m}(E, \vec{k}_{\parallel}) + \psi_{n,m}(E, \vec{k}_{\parallel})]}, \quad (4)$$

where $\phi_{n,m} = [(R-1/2)n + (S+1/2)m]2k_{\perp}(E, \vec{k}_{\parallel})d$, with d the interplanar distance. The plane indices R, S in the Fourier expansion (4) have been shifted by $-1/2$ and $+1/2$, respectively, to enforce symmetry (antisymmetry) on the Fourier coefficients $c_{n,m} = c_{m,n} (-c_{m,n})$ in the ferromagnetic (antiferromagnetic) configuration of the magnetic layers. Such a shift is necessary since the form of the Dyson equation (2) implies that we calculate the local Green's function in the atomic plane immediately to the left of the cleavage plane. It follows that, depending on whether the configuration of the magnetic layers is parallel or antiparallel, the polarization in the connected trilayer satisfies $P(R, S) = \pm P(S+1, R-1)$.

Substituting the Fourier expansion (4) in Eq. (3), we obtain

$$P(R, S) = \frac{\hbar}{2N_{\parallel}} \text{Im} \sum_{n,m} \sum_{\vec{k}_{\parallel}} \int_{-\infty}^{E_F} |c_{n,m}(E, \vec{k}_{\parallel})| \times e^{i[\phi_{n,m}(E, \vec{k}_{\parallel}) + \psi_{n,m}(E, \vec{k}_{\parallel})]} dE. \quad (5)$$

Since the dependences of the polarization on the distance R from the ferromagnet-spacer interface and on the spacer thickness N are now contained entirely in the phase factor $\phi_{n,m}$, Eq. (5) is in a form to which the stationary phase approximation is readily applicable (see Ref. 6). We first note that the polarization at the center of an infinitely thick nonmagnetic spacer must vanish. It follows that $c_{0,0} = 0$, i.e., the Fourier expansion (5) does not involve a constant term. All the terms in Eq. (5) contain, therefore, an imaginary ex-

potential which, for large R and S , oscillates rapidly as a function of E and \vec{k}_{\parallel} , leading to cancellations in the energy and \vec{k}_{\parallel} -space integrals. Both the energy and \vec{k}_{\parallel} -space integrals can, therefore, be evaluated using the stationary phase

approximation. The evaluation of such integrals is described in Ref. 6 and it is easy to show that each stationary point of the spacer Fermi surface makes the following contribution to the local polarization:

$$P(R, N) = -\frac{\hbar A}{8\pi N_{\parallel}} \text{Re} \sum_{n,m} \frac{\tau m^* |c_{n,m}| e^{i\{[(n-m)(R-1/2)+mN]2k_{\perp}d + \psi_{n,m}\}}}{d|(n-m)(R-1/2)+mN| \{ \partial\psi_{n,m}/\partial E + 2d[(n-m)(R-1/2)+mN] \partial k_{\perp}/\partial E \}}, \quad (6)$$

where A is the surface area of the trilayer and we have reverted from the variable S to the spacer layer thickness N ($N=R+S$). The quantity $m^* = |(\partial^2 k_{\perp}/\partial k_x^2)(\partial^2 k_{\perp}/\partial k_y^2)|^{-1/2}$ is the curvature of the spacer Fermi surface at the stationary point \vec{k}_{\parallel}^0 , $\tau = i$ when the arguments in the two Gaussian integrals are positive, $\tau = -i$ when they are negative, and $\tau = 1$ when the arguments have opposite signs. We recall that the perpendicular wave vector k_{\perp} , Fourier coefficients $c_{n,m}$, their phase $\psi_{n,m}$, and all the derivatives in Eq. (6) are evaluated at $E=E_F$ and at the stationary point $\vec{k}_{\parallel} = \vec{k}_{\parallel}^0$. When there is more than one stationary point, the contributions of all such points to the polarization need to be added up.

The stationary phase formula (6) for the induced spin polarization resembles closely the analytic formula for coupling obtained in the quantum well theory of oscillatory exchange coupling.⁶ As in the case of coupling, the induced polarization oscillates with periods $p = \pi/k_{\perp}^0$ that are determined by the extremal radii k_{\perp}^0 of the bulk spacer Fermi surface. The oscillation amplitude is governed by the curvature m^* of the spacer Fermi surface, and by the magnitude $|c_{n,m}|$ of the Fourier coefficients of the spectral density. The latter depends on the degree of confinement of electrons in the spacer quantum well. The rate of decay is determined by the inverse Fermi velocity $\partial k_{\perp}/\partial E$ and the energy derivative of the phase of the Fourier coefficients $\partial\psi_{n,m}/\partial E$. All these factors are common to the induced polarization and oscillatory exchange coupling, which is natural since the two effects are, of course, closely related. However, the fundamental difference between the induced polarization and oscillatory exchange coupling is that the polarization depends in an oscillatory manner both on the spacer thickness N and on the distance R from the ferromagnet spacer interface whereas the coupling is an oscillatory function of the spacer thickness only.

We now turn to the dependences of the induced spin polarization on the distance R from the ferromagnet-spacer interface and on the spacer layer thickness N . To clarify these dependences, some preliminary discussion of the behavior of the Fourier coefficients $c_{n,m}$ is required. We recall that $c_{0,0} = 0$, which is due to the fact that the polarization vanishes at the center of an infinitely thick spacer. Using a straightforward generalization of the arguments given in Ref. 23 for the case of oscillatory exchange coupling, one can further prove that $c_{n,n}$, $c_{n,n+1}$, and $c_{n+1,n}$ are the only nonzero coefficients in the Fourier expansion of the spectral density. In addition, $c_{n,m} = c_{m,n}$ is obtained in the ferromagnetic case

and $c_{n,m} = -c_{m,n}$ holds in the antiferromagnetic case. We shall refer to these results as selection rules for $c_{n,m}$.

To understand the physical significance of the selection rules for $c_{n,m}$, consider the spin polarization induced in a semi-infinite nonmagnetic metal in contact with a semi-infinite ferromagnet. This situation is described by Eq. (6) in the limit $N \rightarrow \infty$, in which case the trilayer reduces to two noninteracting interfaces. It is obvious from simple physical considerations that the induced polarization is nonzero in the vicinity of the interfaces. It is clear from Eq. (6) that, for $N \rightarrow \infty$, nonzero polarization arises only from the terms with $m=0$. Combining this result with the above selection rules for $c_{n,m}$, we find that the polarization induced by an isolated interface is governed by a single Fourier component $c_{0,-1}$ (or $c_{-1,0}$), for each extremal point of the spacer FS. (Negative values of the index n occur because of the form chosen for the Fourier expansion of the spin density [Eq. (4)].) This is clearly the expected Ruderman-Kittel-Kasuya-Yosida (RKKY) or Friedel oscillation of the spin density. It should be noted, however, that RKKY cannot predict the correct amplitude of the induced polarization since it depends on a mismatch between the ferromagnet-spacer potentials at the interface, i.e., on the details of the band structure which are reflected in the magnitude of $c_{0,-1}$ ($c_{-1,0}$).

For finite spacer thickness (trilayer), interference of electron waves reflected from the right and left interfaces occurs and higher-order non-RKKY components $c_{n,m}$ come into play. The stationary phase formula (6) allows us to study the dependence of the polarization on the distance R from an interface for a fixed spacer thickness N , or the dependence on N for a fixed R . Since $c_{n,n} \neq 0$ holds in the ferromagnetic configuration, the diagonal terms $n=m$ in Eq. (6) may lead to a bias (positive or negative) in the R dependence of the polarization. The bias, which occurs only in the ferromagnetic configuration, is determined by the spacer thickness N and is entirely due to non-RKKY contributions. Conversely, since $c_{n,0} \neq 0$, there is a bias in the N dependence of the polarization and the bias is now determined by the position of the plane R where the polarization is observed. It should be noted that a bias in the N dependence may occur both in the ferromagnetic and antiferromagnetic configurations. Finally, as in the case of oscillatory exchange coupling,⁶ the presence of the term $\partial\psi_{n,m}/\partial E$ in the denominator in Eq. 6 has the effect that the expected inverse square law for the decay of the polarization is not always obeyed. For $\partial\psi_{n,m}/\partial E \neq 0$, deviations from the inverse square law may occur even for an isolated interface where one would normally expect the usual RKKY dependence $\propto 1/R^2$.

We now illustrate all these general features by calculating the induced polarization in a Co/Cu/Co trilayer grown in the (001) direction. The Co/Cu/Co system was chosen for two reasons. Firstly, it allows us to test the accuracy of our analytical stationary phase calculation of the induced polarization for a realistic system. The second reason is that the polarization induced in the Cu spacer is highly relevant to the oscillatory exchange coupling we have already calculated for this system.⁶

We consider N (001) atomic planes of Cu sandwiched between two semi-infinite layers of ferromagnetic fcc Co. A small lattice mismatch between Cu and Co is neglected. The Co/Cu interfaces in the trilayer are assumed to be perfect and we use the same tight-binding parametrization of the band structure of the Co/Cu/Co trilayer as in our previous calculation⁶ of the oscillatory exchange coupling. The reader is referred to Ref. 6 for details. We merely mention here that our tight-binding parameters were obtained from fits to an *ab initio* band structure of bulk Cu made by Papaconstantopoulos²⁴ and from our own fits to the band structure of Janak *et al.*²⁵ for bulk ferromagnetic fcc Co. Such a parametrization is expected to be accurate only well away from the interfaces. However, in the case of Co/Cu(001) considered here, LMTO calculations²⁶ show that it is an excellent approximation to use bulk Co and Cu potentials right up to the interfaces. The fits are based on s , p , and d orbitals and hopping up to second nearest neighbors. It follows that the hopping matrix t , the surface Green's functions g , and the trilayer Green's functions G in Eqs. (1) and (2) are all 18×18 matrices. The trilayer Green's functions were constructed following the general strategy outlined earlier. The procedure for a multiorbital band structure is described in detail in Refs. 6,22. We adopted the method of Ref. 22 to determine the Green's functions G^\uparrow and G^\downarrow .

The numerical calculation of the total spin polarization per atom $P(R, N)$ proceeds by direct numerical evaluation of Eq. (1). The energy integral is performed in the complex plane and the \vec{k}_\parallel -space sum over the two-dimensional (2D) Brillouin zone. Typically, 40 energy points and up to 250 000 \vec{k}_\parallel points in the 2D Brillouin zone are needed to achieve convergence.

In Fig. 1 we show the polarizations induced in a Cu layer of $N=21$ atomic planes for the ferromagnetic (a) and antiferromagnetic (b) configurations of the Co layers. The broken curves denote the numerical results computed for noninteger thicknesses of the Cu spacer, while the circles indicate the physically meaningful values of the polarization at integer numbers of atomic planes. For this particular value of the spacer thickness, the bias of the polarization is clearly visible in the ferromagnetic configuration.

We now discuss the stationary phase calculation of the induced polarization. This proceeds by evaluation of Eq. (6). We recall that the right-hand side of this equation is evaluated at the stationary points \vec{k}_\parallel^0 of the perpendicular wave vector k_\perp and at the Fermi energy E_F . Since the Fermi surface of Cu has a single sheet in the layer growth direction, the stationary points coincide with the stationary points of the bulk Cu Fermi surface in the [001] direction, i.e., they are identical with the stationary points that govern oscillatory exchange coupling.^{27,6} There are two such points (in the ir-

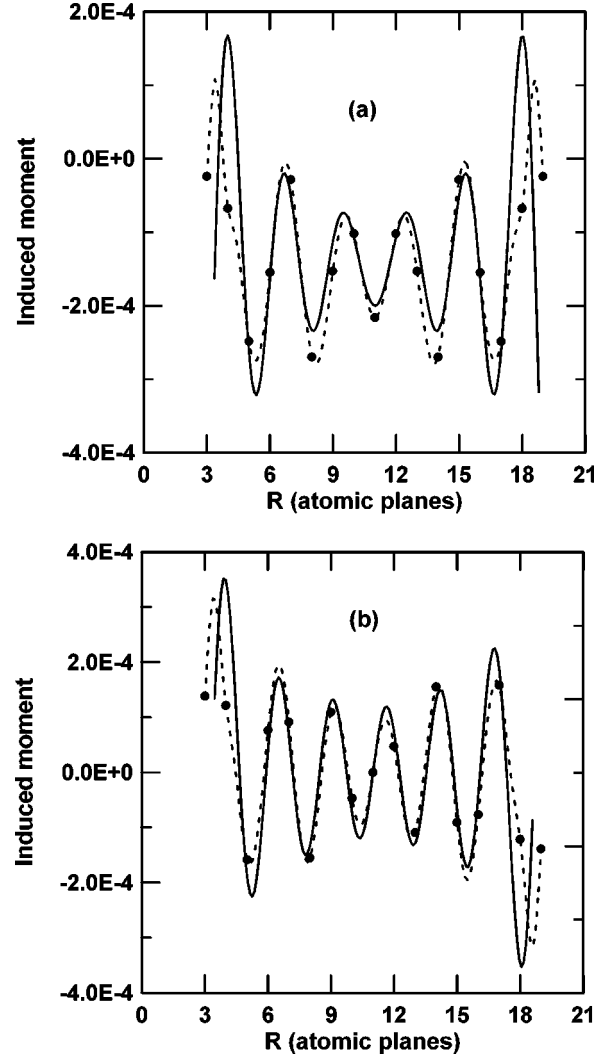


FIG. 1. Dependence of the moment per surface atom induced in the Cu spacer on the distance R from the left Co/Cu interface (in units of $\hbar/2$). The solid circles (broken curves) are the results obtained from a direct numerical evaluation of Eq. (1). The solid curves are the stationary phase results calculated from Eq. (6). (a) Ferromagnetic configuration; (b) antiferromagnetic configuration.

reducible segment of the Brillouin zone) traditionally referred to as the belly [i.e., the Γ point $\vec{k}_\parallel^b = (0,0)$], and the neck [which occurs at $\vec{k}_\parallel^n d = (2.53, 2.53)$].

We begin the evaluation of Eq. (6) with the terms that depend on the Cu Fermi surface only. These are the oscillation period $p = \pi/k_\perp^0$ (measured in numbers of atomic planes), Fermi surface curvature m^* , the ‘‘inverse Fermi velocity’’ $\partial k_\perp / \partial E$, and the factor τ . The values of all these parameters for the belly and neck extrema of the Cu Fermi surface are given in Table I.

The next ingredient is the calculation of the Fourier coefficients $|c_{n,m}|$ and their phases $\psi_{n,m}$. The Fourier coefficients depend on the degree of confinement of electrons in the Cu quantum well⁶ and it will be seen that they are the most important factor that determines the amplitude of polarization oscillations. The Fourier coefficients are defined in the expansion of the (complex) local density of states ρ , via Eq. (4), and can be determined by one of two methods. The

TABLE I. Cu Fermi surface parameters.

k_{\parallel}^0	Period p (number of atomic planes)	m^* (\AA^{-1})	$\partial k_{\perp} / \partial E$ ($\text{Ry}\text{\AA}$) -1	τ
Belly	5.7	0.393	-1.583	-i
Neck	2.6	0.298	-2.057	1

first method is numerical and relies on evaluating $\rho(R,S)$ over a uniform two-dimensional grid in the (R,S) space and then taking a fast Fourier transform. It should be noted that this method requires the knowledge of $\rho(R,S)$ for fractional values of R and S , which means that we need to construct our Green's functions by the method of Ref. 22. The second method is analytical and is very similar to that used in the Fourier analysis of the oscillatory exchange coupling. The method is described in detail in Ref. 23. We merely point out that, using the analytical approach, it can be proved rigorously that all the Fourier coefficients $c_{n,m}$ are related and can be calculated analytically from the Hamiltonian matrix elements. Moreover, one can further prove that $c_{n,n}$, $c_{n,n+1}$, and $c_{n+1,n}$ are the only nonzero coefficients. The selection rules and the actual values of the Fourier coefficients are confirmed by the numerical fast Fourier transform method. Tables II and III give the values at the belly and neck extrema of the modulus, argument, and energy derivative of the argument of some of the lowest Fourier coefficients in the ferromagnetic (FM) and antiferromagnetic (AF) configurations.

Armed with the Cu Fermi surface parameters and the Fourier coefficients, it is a straightforward matter to reconstruct from Eq. (6) the stationary phase contributions to the induced polarization at the belly and neck extrema. In Figs. 2(a) and 2(b) we show the separate contributions to the total polarization induced in Cu in the ferromagnetic and antiferromagnetic configurations arising from the belly and the four neck extrema. The dependence of the polarization on the distance R from the Co/Cu interface is shown again for a Cu layer of $N=21$ atomic planes. It can be seen that the neck contribution oscillates with a short period of about 2.6 atomic planes and the belly contribution has a long period of 5.7 atomic planes. In the FM configuration, there is a strong

TABLE II. Fourier coefficients at the belly extremum in the FM and AF configurations.

$c_{n,m}$	$ c $	ψ	$\partial\psi/\partial E$
$c_{0,-1}^{\text{FM}}$	1.103×10^{-2}	0.3015	9.153
$c_{-1,0}^{\text{FM}}$	1.103×10^{-2}	0.3015	9.153
$c_{-1,-1}^{\text{FM}}$	2.145×10^{-2}	-1.421	8.231
$c_{-1,-2}^{\text{FM}}$	6.458×10^{-4}	-3.137	6.538
$c_{-2,-1}^{\text{FM}}$	6.458×10^{-4}	-3.137	6.538
$c_{-2,-2}^{\text{FM}}$	8.451×10^{-4}	1.436	4.128
$c_{0,-1}^{\text{AF}}$	1.103×10^{-2}	-2.840	9.153
$c_{-1,0}^{\text{AF}}$	1.103×10^{-2}	0.301	9.153
$c_{-1,-2}^{\text{AF}}$	2.112×10^{-4}	-0.020	9.718
$c_{-2,-1}^{\text{AF}}$	2.112×10^{-4}	3.121	9.718
$c_{-2,-3}^{\text{AF}}$	4.044×10^{-6}	2.800	10.282
$c_{-3,-2}^{\text{AF}}$	4.044×10^{-6}	-0.341	10.282

TABLE III. Fourier coefficients at the neck extremum in the FM and AF configurations.

$c_{n,m}$	$ c $	ψ	$\partial\psi/\partial E$
$c_{0,-1}^{\text{FM}}$	0.2778	-0.9445	61.457
$c_{-1,0}^{\text{FM}}$	0.2778	-0.9445	61.457
$c_{-1,-1}^{\text{FM}}$	2.3858	-0.1178	117.338
$c_{-1,-2}^{\text{FM}}$	0.2871	0.6203	177.235
$c_{-2,-1}^{\text{FM}}$	0.2871	0.6203	177.235
$c_{-2,-2}^{\text{FM}}$	2.3645	1.3500	236.586
$c_{0,-1}^{\text{AF}}$	0.2778	2.197	61.457
$c_{-1,0}^{\text{AF}}$	0.2778	-0.944	61.457
$c_{-1,-2}^{\text{AF}}$	2.970×10^{-2}	-1.407	119.586
$c_{-2,-1}^{\text{AF}}$	2.970×10^{-2}	1.735	119.586
$c_{-2,-3}^{\text{AF}}$	3.175×10^{-3}	1.272	177.715
$c_{-3,-2}^{\text{AF}}$	3.175×10^{-3}	-1.869	177.715

bias in the case of the short period. This bias is due to the fact that the Fourier coefficients $c_{n,n}$ are nonzero and large.

The amplitude of the short period contribution is a factor of about 20 larger than that of the long period oscillation, both in the ferromagnetic and antiferromagnetic configurations. The physical mechanism which causes such a large difference in the neck and belly amplitudes is the same as for oscillatory exchange coupling, i.e., full confinement of the minority-spin carriers at the Cu Fermi surface necks.⁶ This is also the reason why the energy derivative of the phase $\partial\psi/\partial E$ is so large at the neck extremum.⁶ A large derivative $\partial\psi/\partial E$ has the effect that the initial decay of the polarization amplitude as a function of the distance R from the interface is slower than the usual inverse square law. This is easier to see in Fig. 2(b) since, in the antiferromagnetic configuration, the polarization oscillates about zero. In fact, it can be seen from Eq. (6) that for large $\partial\psi/\partial E$, the initial dependence of the polarization on the distance from the Co/Cu interface is $\propto 1/R$. Similarly, the initial dependence of the polarization on the Cu layer thickness is $\propto 1/N$. This is in agreement with the experimental results of Samant *et al.*¹⁷ For a Cu layer of 21 atomic planes, the calculated induced moment at the center of the Cu layer is $\approx 10^{-4} \mu_B$. This is consistent with the results of first-principle calculations of Ref. 17 which give $\approx 10^{-3} \mu_B$ for a Cu layer of 7 atomic planes. It should be also noted that the anomalous decay of the polarization in the Co/Cu (001) system invalidates any attempts to fit numerical results to the conventional $\propto 1/R^2$ law (see, e.g., Ref. 18). The same comment applies to the analysis of any past and future experimental data, which must be based on Eq. (6). On the other hand, the derivative $\partial\psi/\partial E$ is small at the belly and, therefore, the amplitude of the belly oscillation obeys the usual RKKY dependence $\propto 1/R^2$.

It is also important to note that, at the neck extremum in the FM configuration, the higher harmonic Fourier coefficients have roughly the same magnitude as the fundamental. The contribution from the non-RKKY terms to the total induced moment is, therefore, large in the case of Co/Cu. It follows that, for Co/Cu, the RKKY contribution from $c_{0,-1}$ and $c_{-1,0}$ alone is a poor approximation to the full stationary phase result (6). Niklasson *et al.*¹⁹ separated numerically the contribution of the non-RKKY terms to the total induced

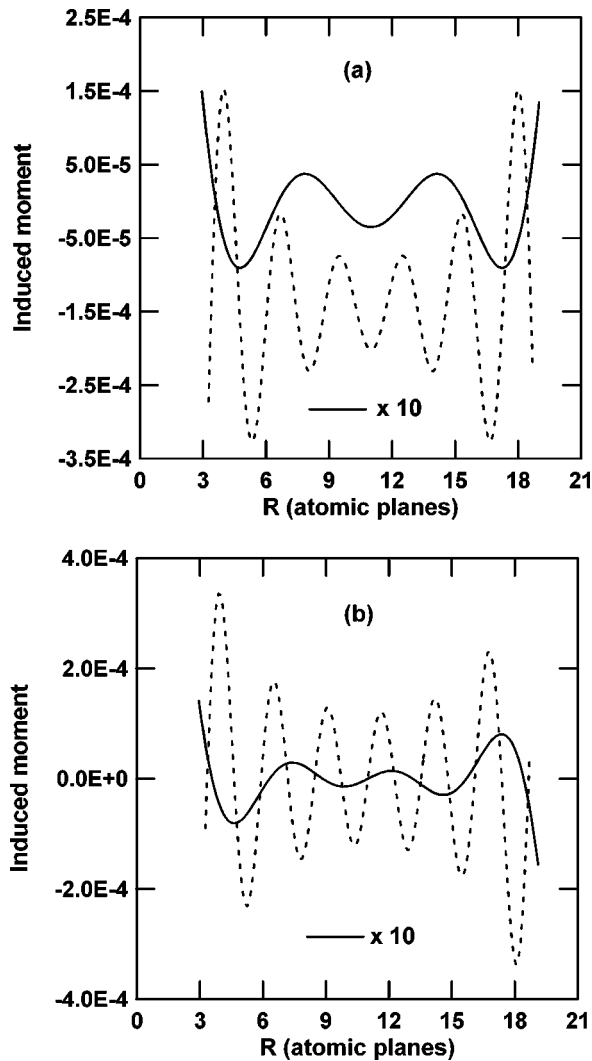


FIG. 2. Contributions to the induced moment (in units of $\hbar/2$) arising from the belly (solid curve) and neck (broken curve) extrema of the Cu Fermi surface. (a) Ferromagnetic configuration; (b) antiferromagnetic configuration. The belly contribution has been multiplied by a factor 10.

moment for a bcc Fe/Cu trilayer. They found that the non-RKKY contribution for the Fe/Cu system is relatively small. This is in contrast to Co/Cu where the non-RKKY contributions to the oscillation amplitude at the center of the Cu layer is more than 25% of the total. More importantly, the large bias seen in Fig. 1 is due entirely to the non-RKKY terms. To see how this bias depends on the spacer thickness, we

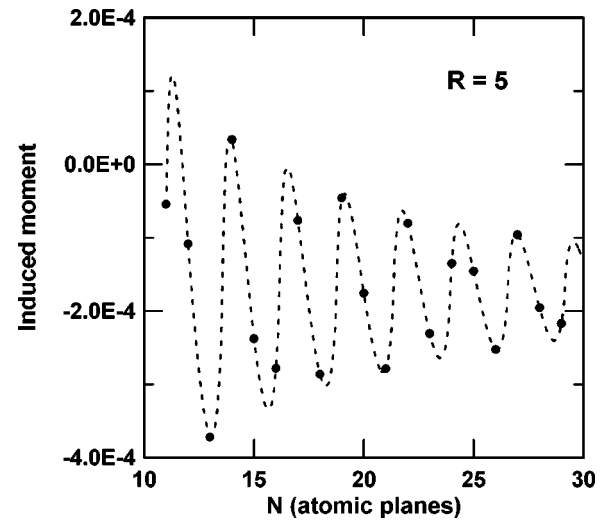


FIG. 3. Dependence of the induced moment (in units of $\hbar/2$) on the Cu spacer thickness at $R=5$, in the ferromagnetic configuration.

plot in Fig. 3 the stationary phase evaluation of the induced moment as a function of the Cu spacer thickness, for the ferromagnetic configuration.

Finally, we return to Figs. 1(a) and 1(b) to compare the numerical results for the total spin polarization with the stationary phase reconstruction. We recall that both the numerical and stationary phase calculations were performed at zero temperature and for $N=21$ atomic planes of Cu sandwiched between two semi-infinite slabs of ferromagnetic Co. The broken curves in Figs. 1(a) and 1(b) denote the numerical results and the solid curves are the stationary phase reconstructions in the ferromagnetic (a) and antiferromagnetic (b) configurations of the trilayer. Despite the relatively small thickness of the Cu layer, there is excellent agreement in amplitude, period, and phase for $5 < R < 16$, which corresponds to the regime in which the stationary phase approximation is valid. Naturally, the asymptotic stationary phase formula fails near the ferromagnet-spacer interface where a numerical *ab initio* calculation is required. The induced polarization is dominated by the short period contribution from the neck and, as already discussed, contains a strong bias in the FM configuration.

The authors thank Dr. J. d'Albuquerque e Castro for stimulating discussions. The support of the Engineering and Physical Sciences Research Council (EPSRC U.K.) and of the Brazilian Academy of Sciences is gratefully acknowledged.

¹S. S. P. Parkin, N. More, and K. P. Roche, Phys. Rev. Lett. **64**, 2304 (1990).

²D. M. Edwards and J. Mathon, J. Magn. Magn. Mater. **93**, 85 (1991); D. M. Edwards, J. Mathon, R. B. Muniz, and M. S. Phan, Phys. Rev. Lett. **67**, 493 (1991).

³D. M. Edwards, J. Mathon, R. B. Muniz, and M. S. Phan, J. Phys.: Condens. Matter **3**, 4941 (1991).

⁴J. Mathon, M. Villeret, and D. M. Edwards, J. Phys.: Condens. Matter **4**, 9873 (1992).

⁵J. Mathon, M. Villeret, R. B. Muniz, J. d'Albuquerque e Castro, and D. M. Edwards, Phys. Rev. Lett. **74**, 3696 (1995).

⁶J. Mathon, M. Villeret, A. Umerski, R. B. Muniz, J. d'Albuquerque e Castro, and D. M. Edwards, Phys. Rev. B **56**, 11 797 (1997).

⁷A. T. Costa, J. d'Albuquerque e Castro, R. B. Muniz, M. S. Ferreira, and J. Mathon, Phys. Rev. B **55**, 3724 (1997).

⁸J. Kudrnovsky, V. Drchal, I. Turek, and P. Weinberger, Phys. Rev. B **50**, 16 105 (1994).

- ⁹V. Drchal, J. Kudrnovsky, I. Turek, and P. Weinberger, Phys. Rev. B **53**, 15 036 (1996).
- ¹⁰P. Lang, L. Nordström, R. Zeller, and P. H. Dederichs, Phys. Rev. Lett. **71**, 1927 (1993).
- ¹¹L. Nordström, P. Lang, R. Zeller, and P. H. Dederichs, Phys. Rev. B **50**, 13 058 (1994).
- ¹²P. Lang, L. Nordström, K. Wildberger, R. Zeller, P. H. Dederichs, and T. Hoshino, Phys. Rev. B **53**, 9092 (1996).
- ¹³*An Introduction to the Electronic, Magnetic and Structural Properties*, Vol. 1 of *Ultrathin Magnetic Structures*, edited by J. A. C. Bland and B. Heinrich (Springer, Berlin, 1994).
- ¹⁴J. E. Ortega and F. J. Himpsel, Phys. Rev. Lett. **69**, 844 (1992).
- ¹⁵J. E. Ortega, F. J. Himpsel, G. J. Mankey, and R. F. Willis, Phys. Rev. B **47**, 1540 (1993).
- ¹⁶P. Segovia, E. G. Michel, and J. E. Ortega, Phys. Rev. Lett. **77**, 3455 (1996).
- ¹⁷M. G. Samant, J. Stöhr, S. S. P. Parkin, G. A. Held, B. D. Hermsmeier, F. Herman, M. van Schilfhaarde, L. C. Duda, D. C. Mancini, N. Wassdahl, and R. Nakajima, Phys. Rev. Lett. **72**, 1112 (1994).
- ¹⁸L. Nordström and D. J. Singh, J. Appl. Phys. **79**, 4515 (1996).
- ¹⁹A. M. N. Niklasson, S. Mirbt, H. L. Skriver, and B. Johansson, Phys. Rev. B **53**, 8509 (1996).
- ²⁰S. Pizzini, A. Fontaine, Ch. Giorgetti, E. Dartyge, J. F. Bobo, M. Piecuch, and F. Baudelet, Phys. Rev. Lett. **74**, 1470 (1995).
- ²¹Q. Y. Jin, Y. B. Xu, H. R. Zhai, C. Hu, M. Lu, Q. S. Bie, Y. Zhai, G. L. Dunifer, R. Naik, and M. Ahmad, Phys. Rev. Lett. **72**, 768 (1994).
- ²²A. Umerski, Phys. Rev. B **55**, 5266 (1997).
- ²³A. Umerski (unpublished).
- ²⁴D. A. Papaconstantopoulos, *Handbook of The Band Structure of Elemental Solids* (Plenum, New York, 1986).
- ²⁵V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, Oxford, 1978).
- ²⁶J. Kudrnovsky, V. Drchal, I. Turek, M. Sob, and P. Weinberger, Phys. Rev. B **53**, 5125 (1996).
- ²⁷P. Bruno and C. Chappert, Phys. Rev. Lett. **67**, 1602 (1991); Phys. Rev. B **46**, 261 (1992).