Temperature dependence of the interlayer exchange coupling in magnetic multilayers: An *ab initio* approach

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The temperature dependence of interlayer exchange coupling (IEC) is studied theoretically within the asymptotic theory with preasymptotic corrections included, and by employing an *ab initio* approach based on the Green function formulation of the IEC. In this paper an efficient method for calculating integrals involving the Fermi-Dirac distribution by representing the occurring integrands by a sum of complex exponentials is discussed. In particular a method which allows us to extract separately the temperature-dependence of the short-period (SPO) and long-period (LPO) oscillations in the case of Co/Cu/Co(001) trilayers from computed values is suggested. Furthermore, a detailed discussion of predictions of asymptotic theory is given. It is found that in the limit of a large spacer thickness N *ab initio* calculations confirm the results of asymptotic theories for SPO for a variety of trilayer geometries, namely, that the oscillation amplitudes depend on the temperature T as $cNT/\sinh(cNT)$. On the other hand, for the case of the LPO this simple form does not apply. We explain this behavior by large preasymptotic corrections necessary for the LPO. The combined effect of the temperature and the disorder in the spacer is also discussed. [S0163-1829(99)03234-8]

I. INTRODUCTION

The oscillatory interlayer exchange coupling (IEC) between magnetic layers separated by a nonmagnetic spacer has attracted considerable attention in the literature (see Refs. 1–3 for recent reviews on this subject). The physical origin of such oscillations is attributed to quantum interferences due to a spin-dependent confinement of electrons in the spacer. The periods of the coupling oscillations with respect to the spacer thickness can be correlated to the geometry of the spacer Fermi surface, a relation that has been used in numerous experiments. First-principles formulations of the IEC, which are not limited by model-like[2] or semiempirical[3] approaches have appeared recently. They can be divided into two groups, namely, direct evaluations by subtracting the total energies of the parallel and antiparallel orientation of magnetizations in the magnetic layers[4] or direct calculations of the IEC energies by using the magnetic force theorem.[5] The present approach[6,7] belongs to the latter group by making systematic use of surface Green functions which in turn not only allow to determine the IEC in a fast and reliable manner (the numerical effort scales linearly with the number of layers in the system), but also facilitate an extension to disordered systems.

Up to now there are very few studies of the temperature dependence of the IEC,[2,8] a systematic study on an *ab initio* level and a verification of conclusions of model theories is missing entirely. This is very important as a reliable determination of the oscillation amplitude is still a challenge to the experiment, not to mention the temperature dependence. Under such circumstances *ab initio* calculations play an extremely important role because they serve as a kind of numerical experiment that can be used to test model theories under well defined conditions which are not attainable in experiments.

The temperature dependence of the IEC can be ascribed to two different mechanisms: (i) Thermal excitations of electron-hole pairs across the Fermi level as described by the Fermi-Dirac function with electron-phonon and electron-magnon interactions supposingly being less important. (ii) Thermal excitations of spin waves in magnetic slabs and particularly at their interfaces reducing the interfilm exchange. This mechanism was discussed on a model level using arguments based on statistical mechanics for a Heisenberg model, see Ref. 9, leading to $1-a(T/T_C)^{3/2}$ dependence of the IEC.

In this paper we limit ourselves to temperature variations of the IEC caused by the Fermi-Dirac statistics. In this case the temperature dependence of the IEC can be evaluated either analytically or numerically. The analytical approach assumes the limit of a large spacer thickness, for which all the oscillatory contributions to the energy integral cancel out with exception of those at the Fermi energy. The energy integral is then evaluated by a standard saddle-point method.

The numerical approach, in which the integrals containing the Fermi-Dirac distribution function as well as the integral over the wave vectors are computed directly, is in principle exact, not limited by the thickness or any assumptions concerning the phase of the integrand, however, it may be numerically very demanding, in particular for low temperatures. In this paper we develop an efficient numerical method for reliably determining the temperature dependence over the whole relevant temperature range including low temperatures. Realistic multilayers usually exhibit more than one period, e.g., the prototype multilayer Co/Cu/Co(001) has short-period oscillations (SPO) as well as long-period (LPO) oscillations. As compared to the SPO, the LPO are usually more robust with respect to interface imperfections. The temperature dependence of the SPO and LPO is generally different. In here we present a method which allows to determine the temperature dependence of the SPO and LPO on an *ab initio* level based on the fact that a discrete Fourier transform of calculated oscillations exhibits usually well separated peaks for the SPO and LPO. This method thus allows to confirm or discard certain conclusions of asymptotic theories. The approach presented here is also applicable to disordered systems with randomness in the spacer, in the magnetic layers, or at interfaces.[10]

II. THEORY

A. Formalism

The multilayer system is considered to consist of three parts, a semi-infinite left and a right magnetic subsystem sandwiching N nonmagnetic atomic spacer layers. The left subsystem contains the semi-infinite nonmagnetic substrate and M_L atomic layers of the left ferromagnetic slab. Similarly, the right subsystem contains the (generally different) semi-infinite nonmagnetic substrate and M_R atomic layers of the right ferromagnetic slab. The magnetic slabs can eventually be semi-infinite. The exchange coupling energy $\mathcal{E}_x(T)$ is given by the difference of the grand canonical potentials for the antiferromagnetic (AF) and ferromagnetic (F) alignments of the magnetic slabs,[7]

$$\mathcal{E}_x(N,T)=\Omega^{\mathrm{AF}}(T)-\Omega^{\mathrm{F}}(T)=\mathrm{Im}\,I(T),$$

$$I(T)=\int_C f(T,z)\Psi(z)dz, \tag{1}$$

where $f(T,z)$ is the Fermi-Dirac distribution function, and

$$\Psi(z)=\frac{1}{\pi}\frac{1}{\Omega_{\mathrm{SBZ}}}\int \mathrm{d}^2\mathbf{k}_\parallel \psi(\mathbf{k}_\parallel,z),$$

$$\psi(\mathbf{k}_\parallel,z)=\mathrm{Tr}[\ln G^{\mathrm{AF}}(\mathbf{k}_\parallel,z)-\ln G^{\mathrm{F}}(\mathbf{k}_\parallel,z)]. \tag{2}$$

The energy integration (contour C) is performed parallel to the real axis, $z=E+i0$, where E extends in principle from $-\infty$ to ∞. The Tr denotes the trace over angular momenta $L=(lm)$, the spin index ($\sigma=\uparrow,\downarrow$), and all atomic layers of the system. The Green functions for the antiferromagnetic and ferromagnetic alignments are denoted as G^{AF} and G^{F}, respectively. The integration over $\mathbf{k}_\parallel$ is restricted to the surface Brillouin zone of area Ω_{SBZ}. We remark that Eq. (2) follows from the Lloyd formula.[11]

B. Model theory

In model type theories the quantity $\psi(\mathbf{k}_\parallel,z)$ in Eq. (2) is approximated by[2]

$$\psi(\mathbf{k}_\parallel,E+i0)\approx\frac{\Omega_{\mathrm{SBZ}}}{\pi}M(\mathbf{k}_\parallel,E)e^{iq(\mathbf{k}_\parallel,E)N}. \tag{3}$$

In this expression, $q(\mathbf{k}_\parallel,E)\equiv k_z^+-k_z^-$ is the difference between the wave vectors of an electron propagating through the spacer in the $+z$ and $-z$ directions (the z axis is taken to be perpendicular to the layer plane; thickness is expressed in units of d, where d is the spacing between atomic planes, and wave vectors are expressed in units of $1/d$). Here a single contribution has been considered; in the general case there are several such contributions, due to multiple bands in the spacer material and to higher harmonics (i.e., higher order terms in an expansion in powers of $e^{iq(\mathbf{k}_\parallel,E)N}$) but the calculation of the various contributions is exactly the same. Thus, for the sake of simplicity, a single contribution is considered here. As explicitly indicated, $q(\mathbf{k}_\parallel,E)$ varies with the energy E and with the in-plane wave vector $\mathbf{k}_\parallel$. The other factor in Eq. (3) is the complex amplitude $M(\mathbf{k}_\parallel,E)$ which depends on the spin-asymmetry of the reflection coefficients at the spacer-ferromagnet interfaces.[2]

The asymptotic approximation is based upon the observation that, because of the strong variation of the Fermi-Dirac function at the Fermi energy, and because of the rapid variation of the exponential factor with E and $\mathbf{k}_\parallel$, the behavior of Eq. (3) at large N is dominated by the contributions of states at the Fermi energy E_{F}, such that the spanning vector of the Fermi surface, $q(\mathbf{k}_\parallel,E)$, is stationary with respect to $\mathbf{k}_\parallel$.[12] In general there may be several such stationary spanning vectors, each of them giving rise to an oscillatory component of the interlayer exchange coupling; the various components are labeled by the index α.

Assuming that in the vicinity of $\mathbf{k}_\parallel^\alpha$ and E_{F} $M(\mathbf{k}_\parallel,E)$ is a smooth function of $\mathbf{k}_\parallel$ and E, it can be approximately replaced by a constant $M_{0\alpha}$

$$M(\mathbf{k}_\parallel,E)\approx M_{0\alpha}. \tag{4}$$

The wave vector $q(\mathbf{k}_\parallel,E)$ can be expanded in the vicinity of $\mathbf{k}_\parallel$ and E_{F} as

$$q(\mathbf{k}_\parallel,E)\approx Q_\alpha+\frac{2(E-E_{\mathrm{F}})}{\hbar v_{F\alpha}}-\frac{(k_x-k_x^\alpha)^2}{\kappa_{x\alpha}}-\frac{(k_y-k_y^\alpha)^2}{\kappa_{y\alpha}}, \tag{5}$$

where $v_{F\alpha}$ is the Fermi velocity, and $\kappa_{x\alpha}$ and $\kappa_{y\alpha}$ are the curvature radii of the Fermi surface at $\mathbf{k}_\parallel^\alpha$ (the x and y axes are chosen so as to eliminate the term proportional to k_xk_y).

Finally, since only the neighborhood of $\mathbf{k}_{\parallel}^{\alpha}$ contributes significantly to the integral, the integration range for k_x and k_y can be formally extended to $(-\infty,+\infty)$. Then, we obtain easily[2]

$$\mathcal{E}_x(N,T)=\sum_{\alpha}\frac{A_\alpha}{N^2}\sin(Q_\alpha N+\Phi_\alpha)t_\alpha(N,T), \tag{6}$$

where the amplitude and the phase are given by

$$A_\alpha e^{i\Phi_\alpha}=\frac{\pi}{2}\hbar v_{F\alpha}(\kappa_{x\alpha})^{1/2}(\kappa_{y\alpha})^{1/2}M_{0\alpha}. \tag{7}$$

The temperature dependence is then given[2] by the function

$$t_\alpha(N,T)=\frac{c_\alpha NT}{\sinh(c_\alpha NT)}, \tag{8}$$

with

$$c_\alpha=\frac{2\pi k_B}{\hbar v_F^\alpha}. \tag{9}$$

The most remarkable result of this analytic approach is that the scaling factor $t(N,T)$ depends on the product of spacer thickness N and temperature T. In the preasymptotic region (small spacer thickness) the functional form of $t(N,T)$ differs from that of Eq. (8) due to a rapid variation of the phase of the integrand of the IEC.[8] In this case preasymptotic corrections are non-negligible.

C. *Ab initio* approach

We employ the tight-binding linear muffin-tin orbital (TB-LMTO) method and the technique of surface Green functions[13,14] to determine $\Psi(z)$. The details can be found in Ref. 7. The integral containing the Fermi-Dirac function in Eq. (1) can be calculated by a standard method based on the Gaussian quadrature along the contour C and a summation over the enclosed Matsubara poles (see, e.g., Ref. 7). Since the Matsubara poles depend on the temperature, the function $\Psi(z)$ has to be evaluated for each temperature under consideration. A new integration method which is described in the Appendix allows to substantially speed up such calculations.

D. Details of calculations

The numerical studies were performed for the (001) direction of a parent fcc lattice[15] corresponding to the experimental lattice spacing of Cu. In each case, the magnetic layers are Co layers, the spacer and the substrate layers are formed by Cu layers (a conventional trilayer geometry). All calculations are based on self-consistent potentials of bulk fcc-Cu and bulk fcc-Co aligned to a common Fermi energy.[16] We have performed self-consistent calculations for Cu at $T=500$ K and found a negligible influence of finite temperatures on the potentials and hence also on the Fermi energy and the shape of the Fermi surface. We neglected a change of magnetic moments in the Co slabs with temperature because the temperatures considered in this study ($T\leqslant 500$ K) are small as compared to the Curie temperature 1360 K of bulk Co. Clearly enough, this approximation is the better the thicker the Co slabs are and may be not justified for a single monolayer Co slabs.

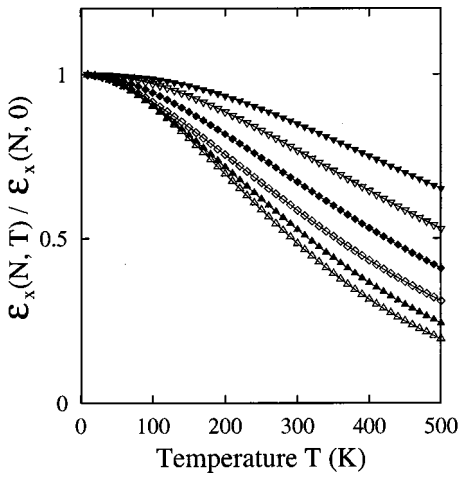

FIG. 1. $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$ as a function of the temperature T for a trilayer consisting of semi-infinite Co(001) slabs sandwiching a fcc-Cu spacer. The different curves refer to different spacer thicknesses N ($N=9$, 14, 19, 24, 29, and 34 from top to bottom).

In order to determine the parameters of the complex exponentials (A3), we evaluated the function $\Phi(y)$ at the 40 Matsubara energies corresponding to $T=25$ K. We found that between 25 and 100 K the results depend only weakly on the actual value of T. Note that such calculations have to be performed only once. The calculations were carried out for spacer thicknesses up to 80 monolayers and for temperatures up to 500 K (in steps 10 K) for different trilayers of Co/Cu/Co(001), namely, for semi-infinite Co slabs, and for finite Co slabs. It is well known[6,5,17] that for thick magnetic slabs the short-period oscillations (SPO) dominate and the contributions from the long-period oscillations (LPO) can be neglected.

III. RESULTS AND DISCUSSION

In model studies[2,3] one typically makes use of the asymptotic theory in order to obtain the temperature dependence of the IEC. Recent papers,[8,18] however, demonstrate that preasymptotic corrections may be quite important in some cases. *Ab initio* theories, similarly to experiment, provide the IEC for a set of spacer thicknesses and temperatures. This in turn requires a sophisticated analysis and visualization of calculated results.

A. The case of a single oscillation period

The simplest way[7,8] of presenting the results is to plot directly $\mathcal{E}_x(N,T)$ as a function of the spacer thickness for a few chosen temperatures. Such a representation is, however, obscured by the standard N^{-2} decay of the oscillation amplitudes and hardly demonstrates more than the simple fact that the oscillations are damped by finite temperatures. Alternatively[8] one can present the ratio $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$, or, more generally, the ratio $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,T_0)$ where T_0 is some chosen temperature. In Fig. 1 the ratio $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$ for a set of spacer thicknesses roughly corresponding to the maxima of $N^2\,\mathcal{E}_x(N,T)$ is plotted. We ob-

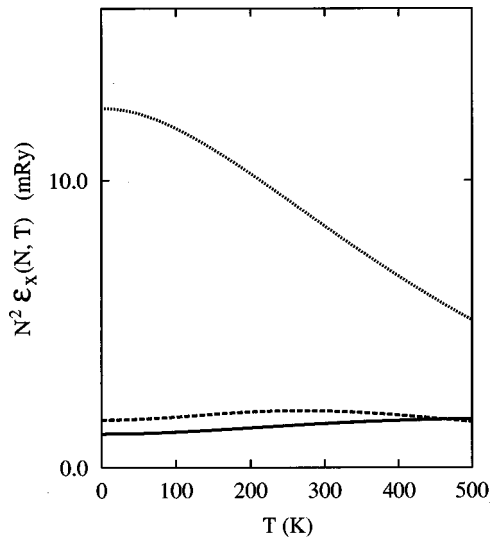

FIG. 2. $N^2\mathcal{E}_x(N,T)$ as a function of the temperature T for a trilayer consisting of semi-infinite Co(001) slabs sandwiching a fcc-Cu spacer. The different curves refer to different spacer thicknesses N: $N=7$ (full line), $N=22$ (dashed line), and $N=19$ (dotted line). The latter case (see also Fig. 1) is used to highlight a different behavior of $N=7$ and $N=22$ cases in comparison with $N=19$, as well as the fact that they correspond to the transient regime between the ferromagnetic and antiferromagnetic coupling.

serve a systematic decrease of the oscillation amplitudes with temperature which, in accordance with the model result in Eq. (8), is more pronounced for thicker spacers. For $N=9$ the decay of the oscillation amplitude with temperature is in close agreement with curve (1) in Fig. 3 of Ref. 8 (semiempirical multiband tight-binding model). It is important to exclude the preasymptotic region and, in particular, to consider only cases with a well defined type of coupling (either ferromagnetic or antiferromagnetic), since otherwise, as illustrated in Fig. 2, one obtains results which can significantly deviate from the expected behavior. In particular, the cases plotted in Fig. 2 correspond to layers close to the transition between the ferromagnetic and the antiferromagnetic coupling, i.e., to the case for which $N^2\,\mathcal{E}_x(N,T)$ is close to zero.

The most important prediction of the model presented in Ref. 2 is that the IEC depends on the product of spacer thickness and temperature, $\zeta=NT$ [see Eq. (8)]. In order to verify this prediction, in Fig. 3 $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$ is plotted as a function of the parameter $x=NT$. It should be noted that each point in the plot represents a separate calculation at a given temperature and spacer thickness. The asymptotic behavior is obtained by restricting the spacer thickness to $N\geqslant 20$ and by explicitly excluding a few cases with very small values of $N^2\,\mathcal{E}_x(N,T)$ (e.g., the case with $N=22$). It is seen that the calculated values of $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$ can be fitted rather well by a least-square fit to the function $\xi/\sinh(\xi)$, $\xi=c\,NT$ with $c=1.95\times10^{-4}\ \mathrm{K}^{-1}$. It is evident from Fig. 3 that for large spacer thicknesses and a numerically determined constant c the model predictions are reasonably well confirmed: The value of $c_S=1.85\times10^{-4}\ \mathrm{K}^{-1}$ reported in Ref. 12, which in turn is based on the use of experimental Fermi surface parameters, is in a rather good agreement with the present result.

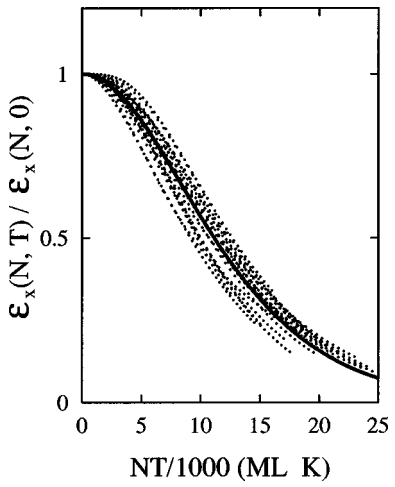

FIG. 3. $\mathcal{E}_x(N,T)/\mathcal{E}_x(N,0)$ plotted as a function of $x=NT$ for a trilayer consisting of semi-infinite Co(001) slabs sandwiching a fcc-Cu spacer. The thick line refers to $\xi/\sinh(\xi)$, $\xi=c\,NT$ with $c=0.000\,195\ \mathrm{K}^{-1}$ as obtained by a least-square fit to the computed data.

B. The case of more than one oscillation period

The mode of analyzing the results as presented in Fig. 3 is inapplicable for the case of more than one oscillation period.[1,12] Below we sketch an alternative visualization based on discrete Fourier transformations, by which various periods corresponding to separated peaks can be distinguished.

In general, the interlayer exchange coupling energy in the asymptotic regime of large spacer thickness can be viewed as a sum of several contributions from nonequivalent extremal vectors $\mathbf{k}_{||}^{\alpha}$ of the spacer Fermi surface (callipers)[2] as given by Eq. (6). We wish to resolve the individual contributions to $\mathcal{E}_x(N,T)$ and then to check the functional form of $t_\alpha(N,T)=f[c_\alpha(x)]$, Eq. (8), where $f(\xi)=\xi/\sinh(\xi)$, $\xi=c_\alpha x$, and $x=NT$, as well as to find the values of the coefficients c_α.

Let us first introduce the auxiliary function

$$\mathcal{F}_x(N,T_{\mathrm{eff}})=N^2\,\mathcal{E}_x\left(N,\frac{T_{\mathrm{eff}}}{N}\right). \tag{10}$$

The interlayer exchange coupling energies $\mathcal{E}_x(N,T)$ are evaluated for the temperatures $T_N=T_{\mathrm{eff}}/N$ that depend on both the fictitious temperature T_{eff} and the number N of spacer layers. The fictitious temperature T_{eff} plays the role of the product NT. The contributions of the individual callipers $\mathbf{k}_{||}^{\alpha}$ to $\mathcal{E}_x(N,T)$ can be identified from the peaks in the discrete Fourier transform

$$F(q,T_{\mathrm{eff}})=\frac{1}{N_2-N_1+1}\sum_{N=N_1}^{N_2}\exp(iqN)\mathcal{F}_x(N,T_{\mathrm{eff}}). \tag{11}$$

By inserting Eqs. (6) and (10) into Eq. (11), we find

$$F(q,T_{\mathrm{eff}})=\sum_{\alpha}J_\alpha(q)f(c_\alpha T_{\mathrm{eff}}), \tag{12}$$

where

TABLE I. Least-square fits of the coefficients c_S and c_L for Co/Cu/Co multilayers with varying thickness M of the Co slabs. The position of the peak of the discrete Fourier transformation is q and Δ is the rms error of the fit. Both short- and long-period oscillations are present for finite Co slabs, while the amplitudes of long-period oscillations are suppressed for semi-infinite Co slabs.

	Short period			Long period		
M	q	Δ	c_S (K^{-1})	q	Δ	c_L (K^{-1})
∞	2.48	0.0003	0.000195			
5	2.48	0.0002	0.000190	1.21	0.0002	0.000275
1	2.43	0.0003	0.000194	0.94	0.1367	0.000249

$$J_\alpha(q)=\frac{1}{N_2-N_1+1}\sum_{N=N_1}^{N_2}\exp(iqN)A_\alpha\sin(Q_\alpha N+\Phi_\alpha) \tag{13}$$

is the contribution of calliper α to the discrete Fourier transform at $T=0$ K. As this quantity has a sharp peak at Q_α, well separated from other peaks at $Q_{\alpha'}$ $(\alpha'\neq\alpha)$, the temperature factor $f_\alpha(T_{\rm eff})$ can be found from Eq. (12) by neglecting the contributions from other callipers, namely,

$$f(c_\alpha T_{\rm eff})\approx\frac{F(q_\alpha,T_{\rm eff})}{F(q_\alpha,0)}. \tag{14}$$

To illustrate this approach, we have performed calculations for $20\leqslant N\leqslant 60$ of spacer layers and for 30 effective temperatures $T_{\rm eff}$. The calculated values of $f(c_\alpha NT)$, Eq. (14), were then fitted by the least-square method to the assumed form, Eq. (8). The quality of the fit as given by the rms error, is displayed in the Table I.

For semi-infinite Co slabs (Fig. 4, Table I) a good-quality fit yields a value of $c_S=1.95\times10^{-4}$ K^{-1}, which is in a good agreement with the value extracted from experimental data and the value corresponding to Fig. 3. Equally good agreement for the c_S of the SPO is found for finite magnetic layers, namely, for the case of the five monolayer slabs (Fig. 5, Table I) and single monolayer slabs (Table I). It should be noted that the values of c_S as determined from different subsets are quite robust, namely, the results for N $10\leqslant N\leqslant 50$ and $20\leqslant N\leqslant 80$ differ only by five percent from those for $20\leqslant N\leqslant 60$.

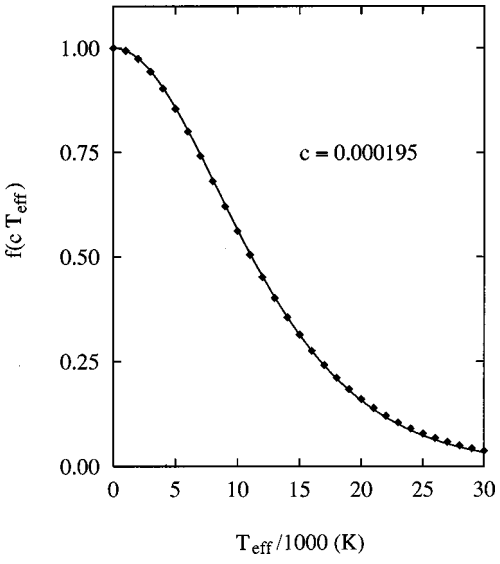

FIG. 4. The function $f(T_{\rm eff})$ for two semi-infinite Co slabs sandwiching a Cu spacer, Eq. (17), calculated as the ratio of the absolute values of the discrete Fourier transformations of $N^2\mathcal{E}_x(N,T_{\rm eff})$ for the subset $N\in 20$–60 and a set of temperatures $T_{\rm eff}$. The calculated values (diamonds) corresponding to the short-period oscillations are shown together with their least-square fits (full line) represented by $f_S(x)=c_S x/\sinh(c_S x)$, $c_S=0.000195$.

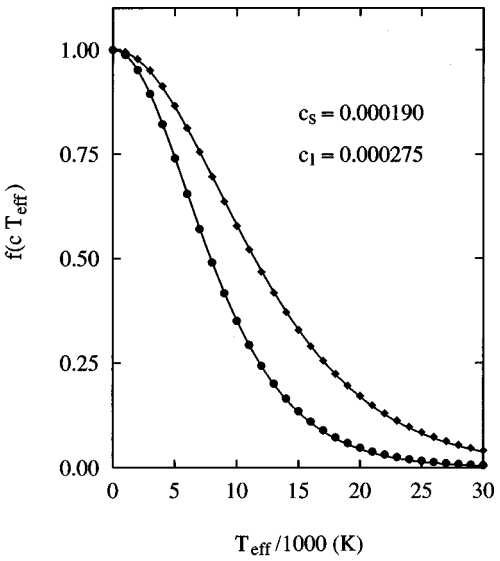

FIG. 5. The function $f(T_{\rm eff})$, Eq. (17), calculated as a ratio of the absolute values of the discrete Fourier transformations of $N^2\mathcal{E}_x(N,T_{\rm eff})$ for the subset $N\in 20$–60 and a set of temperatures $T_{\rm eff}$ for two finite Co slabs each five monolayers thick embedded in a Cu spacer. The calculated values (diamonds and heavy dots) corresponding to the short (S) and long (L) period oscillations, respectively, are shown together with their least-square fits (full lines) represented by $f_\alpha(x)=c_\alpha x/\sinh(c_\alpha x)$, $\alpha=S,L$; $c_S=0.000190$ and $c_L=0.000275$.

The case of the LPO is different. For five monolayer slabs (Fig. 5, Table I), the least-square fit is still of good quality yielding $c_L=2.75\times10^{-4}$ K^{-1}, and is very robust with respect to various subsets of N. This value should be compared with $c_L=1.42\times10^{-4}$ K^{-1} as obtained from using experimental Fermi surface parameters.[12] The case of single monolayer slabs gives a poor quality fit (large rms error, Table I) which also strongly depends on the choice of subsets used for the discrete Fourier transformation. We can thus conclude that the temperature factor $f(c_\alpha NT)$ for the LPO in the single monolayer system differs considerably from the expected functional form, Eq. (8). This, together with the fact that also the period of the LPO depends strongly on the thickness of the Co layer and on the subset N used in the Fourier analysis, is a clear indication of strong preasymptotic corrections as discussed in detail in Refs. 8 and 18.

One source of preasymptotic corrections which has a strong influence on the temperature dependence of the coupling is the variation of $M(\mathbf{k}_\parallel,E)$ with respect to E. If this variation is strong, then it cannot be neglected any longer. As shown in Ref. 18, one then obtains

TABLE II. Least-square fits of the coefficient c_S for semi-infinite Co slabs sandwiching an alloy spacer. The position of the peak of the discrete Fourier transformation is q and Δ denotes the rms error of the fit. Only short-period oscillations are present for semi-infinite Co slabs. The case of ideal Cu spacer is also shown.

	Short period		
spacer	q	Δ	c_S (K^{-1})
Cu	2.48	0.0003	0.000195
$Cu_{85}Ni_{15}$	2.77	0.0052	0.000259
$Cu_{50}Au_{50}$	2.66	0.0132	0.000247
$Cu_{75}Zn_{25}$	2.06	0.0047	0.000200

$$\mathcal{E}_x(N,T)=\sum_\alpha \left[\frac{A_\alpha}{N^2}\sin(Q_\alpha N+\Phi_\alpha) f(c_\alpha NT) + \frac{B_\alpha}{N^3}\cos(Q_\alpha N+\Phi_\alpha) g(c_\alpha NT)\right], \quad (15)$$

where B_α is related to the energy derivative of $M(\mathbf{k}_\parallel,E)$. The temperature dependence of the correction is given by (see Fig. 1 of Ref. 18)

$$g(\xi)=\frac{\xi^2\cosh\xi}{\sinh^2\xi}. \quad (16)$$

As the reflection coefficient of minority electrons with $\mathbf{k}_\parallel = 0$ for thin layers of Co embedded in Cu (001) varies rather strongly with energy (see Refs. 2 and 19), this causes a large departure from the asymptotic behavior for the long period oscillation.

C. Combined effect of the temperature and disorder

The present method is also applicable to the case of disordered samples, in particular, it allows us to study the combined effect of temperature and alloying in the spacer. By employing the vertex-cancellation theorem,[10] a generalization to random alloys is straightforward, namely, only a substitution of the Green functions in Eq. (2) by their configurationally averaged counterparts is needed.[14] With exception of this change the analysis described in the previous sections remains unchanged.

One of the main results of asymptotic theories is that the temperature dependence of the oscillation amplitudes is related to details of the spacer Fermi surface. The spacer Fermi surface can be strongly influenced by alloying because the electron concentration changes and the alloy Fermi surface is modified.[20] The most obvious effect of alloying is the change of the periods of oscillations connected with the change of the corresponding callipers. We refer to a recent paper[21] for more details concerning the semi-infinite Co slabs sandwiching the alloy spacer $Cu_{100-x}M_x$, where $M=$Ni, Au, and Zn. The coefficients c_S for short-period oscillations which for the model of semi-infinite Co slabs also dominate in the case of alloy spacers, are summarized in Table II for three typical alloy spacers. Alloying of the Cu spacer with Ni (Zn) impurities reduces (extends) oscillations periods while the effect of Au atoms is rather small. The temperature dependence is thus again of the form $\xi/\sinh(\xi)$, $\xi=c_S NT$ with values c_S as given in Table II. Disorder leads to a somewhat larger additional damping as compared to the case of a pure Cu spacer (see Table I). In full agreement with the qualitative conclusions in Ref. 21 the damping for a CuZn spacer is smaller as compared to CuNi or CuAu spacers.

IV. CONCLUSIONS

We have investigated the effect of temperature on interlayer exchange coupling assuming that the main mechanism consists in thermal excitations of electron-hole pairs as described by the Fermi-Dirac function. We have used a spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method and the Lloyd formulation of the integrated density of states. The occurring integrals are calculated by means of an efficient method of representing the integrands containing the Fermi-Dirac distribution by a sum of complex exponentials. For a given geometry one has to determine the parameters of the exponentials only once and then the IEC is obtained very quickly and reliably for any reasonable temperature. Our calculations for Co/Cu/Co(001) trilayers confirm a simple functional dependence of the IEC on the product of temperature and spacer thickness, namely, $\mathcal{E}_x(N,T)=\mathcal{E}_x(N,0)\,[\xi/\sinh(\xi)]$, where $\xi=c\,NT$, valid for large N. We found, however, that in the preasymptotic regime and for very small coupling amplitudes the actual temperature dependence can significantly deviate from this simple form. The present study shows a different temperature dependence of the short- and long-period oscillations, the latter decay faster than the former. We have also found that for one monolayer thick magnetic slabs the temperature dependence is more complicated than those predicted by simple models. It should be mentioned that within the present method also the combined effect of temperature and disorder[21] can be studied.

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APPENDIX: NUMERICAL TREATMENT OF THE TEMPERATURE DEPENDENCE

The integral in Eq. (1) can be recast into a more suitable form using the analytic properties of the function $\Psi(z)$, namely, (i) $\Psi(z)$ is holomorphic in the upper half of the complex plane and (ii) $z\Psi(z)\to 0$ for $z\to\infty$, $\mathrm{Im}\,z>0$. Let us define a complex function $\Phi(y)=-i\,\Psi(E_F+iy)$ of a real variable y, $y\geqslant 0$. Then at $T=0$ K,

$$I(0)=\int_0^{+\infty}\Phi(y)dy, \tag{A1}$$

while at $T>0$ K,

$$I(T)=2\pi k_B T\sum_{k=1}^{\infty}\Phi(y_k), \tag{A2}$$

where $y_k=\pi k_B T(2k-1)$ are Matsubara energies and k_B is the Boltzmann constant. In the limit of $T\to 0$, $I(T)\to I(0)$ continuously.

The function $\Psi(z)$ is rapidly oscillating for z just above the real axis and it is strongly damped for z moving deep into the upper half-plane. One can thus expect that the function $\Phi(y)$ can be represented by a sum of a few complex exponentials

$$\Phi(y)\approx F(y),\quad F(y)=\sum_{j=1}^{M}A_j\exp(p_j y), \tag{A3}$$

where the A_j are complex amplitudes and the p_j complex wave numbers ($\mathrm{Re}[p_j]<0$).

The evaluation of $I(T)$ is then straightforward, since the sum over k in Eq. (A2) represents for each p_j from Eq. (A3) a geometrical series. The result is

$$I(T)=-2\pi k_B T\sum_{j=1}^{M}\frac{A_j}{\exp(\pi k_B T p_j)-\exp(-\pi k_B T p_j)}, \tag{A4}$$

which for $T=0$ K gives

$$I(0)=-\sum_{j=1}^{M}\frac{A_j}{p_j}. \tag{A5}$$

The function $\Phi(y)$ attains the values $\Phi_n=\Phi(y_n)$ for y_n, $n=1,\ldots,N$. For a given set $\{\Phi_n\}$, the parameters A_j and p_j can be found by using nonlinear least-square fit methods. Here we present a much simpler, more efficient and reliable method for finding the parameters A_j and p_j in Eq. (A3). Let $z_j=\exp(p_j h)$, then there always exist coefficients B_m, $m=0,1,\ldots,M$, such that

$$\sum_{m=0}^{M}B_m\exp(p_j hm)=\sum_{m=0}^{M}B_m z_j^m=0 \tag{A6}$$

for all $j=1,\ldots,M$, because $M+1$ M-dimensional vectors $(z_1^m,\ldots,z_M^m)$ are always linearly dependent. Let $\{y_n\}$, $n=1,\ldots,N$, $N\geq 2M$, be an equidistant set, i.e.,

$$y_n=y_0+hn,\ n=1,\ldots,N. \tag{A7}$$

The values $F_n=F(y_n)$ then fulfill $(M+1)$-recurrence relations

$$\sum_{m=0}^{M}B_m F_{m+k}=0, \tag{A8}$$

for $1\leq k\leq N-M$, as readily follows by inserting Eqs. (A3) and (A7) into Eq. (A8) and using Eq. (A6),

$$\sum_{m=0}^{M}B_m F_{m+k}=\sum_{j=1}^{M}A_j\exp(p_j[y_0+hk])\sum_{m=0}^{M}B_m\exp(p_j hm)=0. \tag{A9}$$

The coefficients B_m are found from the condition that the recurrence relations (A8) hold also for the function $\Phi(y)$. Without loss of generality we can assume $B_0=1$. In this way we obtain

$$\sum_{m=1}^{M}\Phi_{m+k}B_m=-\Phi_k, \tag{A10}$$

which represents a set of $N-M$ inhomogeneous linear equations for M unknown coefficients B_m. If $N=2M$ these equations can be solved by standard methods. In most cases, however, one wishes to use more function values Φ_m than necessary ($N>2M$) in order to eliminate possible computational errors and to obtain a better fit. Optimized coefficients B_m can be obtained from a *linear* least-square fit, or pseudoinversion[22] of the $[(N-M)\times M]$ matrix of the left-hand side of Eq. (A10). The resulting equations read

$$\sum_{m=1}^{M}\left(\sum_{k=1}^{N-M}\Phi_{i+k}^{*}\Phi_{m+k}\right)B_m=-\sum_{k=1}^{N-M}\Phi_{i+k}^{*}\Phi_i, \tag{A11}$$

where the asterisk denotes a complex conjugate, and $1\leq i\leq M$.

Once the coefficients B_m are known, Eq. (A6) can be solved. The roots z_j can be determined for example as the eigenvalues of the companion matrix.[23] The wave numbers are then determined as $p_j=\log(z_j)/h$. The function $\Phi(y)$ is bounded or even tends to zero for $y\to+\infty$. Consequently, wave numbers with $\mathrm{Re}[p_j]>0$ have to be discarded.

The amplitudes A_j are given by the following set of inhomogeneous linear equations

$$\sum_{j=1}^{M}\exp(p_j y_k)A_j=\Phi_k, \tag{A12}$$

that are solved again directly for $N=2M$, or by a linear least-square fit for $N>2M$,

$$\sum_{j=1}^{M}\sum_{n=1}^{N}\exp[(p_i^{*}+p_j)y_n]A_j=\sum_{n=1}^{N}\exp(p_i^{*}y_n)\Phi_n. \tag{A13}$$

Although we have never encountered such a case in our calculations, Eq. (A6) can have one or more multiple roots (with multiplicities P_j). In such a case basis functions of a more general form, namely, $\{y^{\lambda}\exp(p_j y)\}$, $\lambda=0,1,\ldots,P_j$, have to be considered and Eq. (A13) should be modified accordingly.

The number M of complex exponentials needed to represent $\Phi(y)$ is usually not known in advance. Therefore we have varied M in a broad range, say between 2 and 12, and selected a value that gave the best fit of $\Phi(y)$.

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