Spin waves in ultrathin ferromagnetic overlayers

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The influence of a nonmagnetic metallic substrate on the spin-wave excitations in ultrathin ferromagnetic overlayers is investigated for different crystalline orientations. We show that spin-wave damping in these systems occurs due to the tunneling of holes from the substrate into the overlayer, and that the spin-wave energies may be considerably affected by the exchange coupling mediated by the substrate.

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I. INTRODUCTION

Recent advances in materials growth techniques and precise control of deposition processes have enabled production of multilayers with excellent interfacial quality.[1,2] Presently, it is possible to grow ultrathin magnetic films on a substrate, regulating the film thickness very accurately. Epitaxial films with very well-defined thicknesses, showing virtually no layer thickness fluctuation over macroscopic distances, have been fabricated.[1] The ability to control film thicknesses with such accuracy, together with the freedom to choose different substrates with distinct crystalline orientations, broadens the spectrum of magnetic responses, and makes these systems highly attractive for technological applications.

The magnetic behavior of ultrathin films is strongly affected by spin-wave excitations. Hence, the study of spin waves in these structures is important for understanding their magnetic properties and characteristics. In fact, spin waves in ultrathin films have been extensively studied, both experimentally and theoretically.[3–5] At low temperatures, for instance, the magnetization reduction is basically controlled by long-wavelength spin waves. Thus, measurements of $M(T)$ can provide useful information about spin-wave excitations in low-dimensional magnetic structures. Other experimental techniques such as Brillouin light scattering[6] and ferromagnetic resonance[7] give more direct information about long-wavelength spin-wave excitations, and have been largely used to characterize and study the magnetic behavior of thin films. A good account of some of these experimental methods applied to magnetic thin films can be found in Ref. 8.

Generally, the energy of a long-wavelength spin wave propagating with wave vector $\mathbf{q}$ is given by $E=D(\hat{q})q^2$, where $D(\hat{q})$ is the exchange stiffness constant. In a relatively thin magnetic layer, spin waves are excited with wave vectors $\mathbf{q}_{\parallel}$ parallel to the layer, and for certain crystalline orientations, the spin-wave energies may depend strongly upon the direction of $\mathbf{q}_{\parallel}$,[9] due to lattice anisotropies.

Inelastic neutron-scattering measurements provide access to wave vectors within a broader region around the Brillouin-zone center, but they are more difficult to perform in ultrathin films due to the relatively small scattering volumes involved.[10] More recently, spin-polarized electron energy-loss spectroscopy appears as a promising technique to probe short-wavelength spin waves, and is expected to provide relevant additional information on the magnetic response of thin films.[11]

It has been shown[12] that spin-wave lifetimes in ultrathin ferromagnetic films can be substantially affected by the presence of a nonmagnetic substrate. By considering a monolayer of a strong ferromagnet on a surface of a noninteracting metallic substrate, Phan *et al.*[12] showed that spin waves in the overlayer become critically damped. Such behavior has been attributed to the decaying of spin waves into electron-hole pairs due to the tunneling of holes from the substrate into the magnetic overlayer. The substrate also affects the spin-wave energy, and modifies the region in $q_{\parallel}$ space where it follows a quadratic behavior.

Here we pursue these ideas and investigate the influence of a nonmagnetic substrate in spin-wave excitations in ultrathin ferromagnetic overlayers for different crystalline orientations. We consider a monolayer of a strong ferromagnet both on (100) and (110) surfaces of a semi-infinite nonmagnetic metallic substrate. By artificially reducing the electron hopping between the substrate and the overlayer we explicitly demonstrate that the spin-wave damping is really due to the tunneling of holes from the substrate into the overlayer, as previously pointed out by Phan *et al.*[12] For the (110) overlayer we have found that the spin-wave energies depend upon the $\mathbf{q}_{\parallel}$ direction, but such dependence is much less pronounced than previously found for unsupported monolayers. This is due to the enhancement of the exchange coupling between the local moments in the overlayer mediated by the substrate, which strongly affects the spin-wave energies.

This paper is organized as follows: in Sec. II we briefly review the theory we have used to calculate the spin-wave energies and lifetimes in overlayers. In Sec. III we present our results and discussions, and finally, in Sec. IV, we draw our main conclusions.

II. TRANSVERSE SPIN SUSCEPTIBILITY

The spin-wave spectrum of itinerant ferromagnets can be obtained from the dynamical transverse spin susceptibility

$$\chi^{+-}(\mathbf{q},\omega)=\sum_j \int_{-\infty}^{\infty} dt\, e^{-i\omega t} e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \chi_{ij}^{+-}(t), \quad (1)$$

where $\chi_{ij}^{+-}(t)=\langle\langle S_i^+(t);S_j^-(0)\rangle\rangle$ is the time-dependent transverse spin susceptibility in real space given by the two-particle Green's function

$$\chi_{ij}^{+-}(t)=-i\Theta(t)\langle[S_i^+(t),S_j^-(0)]\rangle. \quad (2)$$

Here, S_i^+ (S_i^-) is the spin raising (lowering) operator at site i, the brackets denote a commutator, $\langle\ldots\rangle$ represents the thermodynamical average, which at zero temperature, reduces to the ground-state expectation value, and $\Theta(t)$ is the usual step function given by

$$\Theta(t)=\begin{cases} 0 & \text{if } t<0 \\ 1 & \text{if } t>0. \end{cases}$$

The exact calculation of $\chi_{ij}^{+-}(t)$ involves the solution of an infinite set of coupled equations that in general is not possible to find. However, the random-phase approximation (RPA) provides a useful decoupling scheme that allows one to solve such equations and obtain the spin-wave energies rather accurately. To find an expression for $\chi_{ij}^{+-}(t)$ within the RPA, we follow Refs. 13 and 14 and define the spin operators

$$S_{ij}^+=a_{i\uparrow}^\dagger a_{j\downarrow},$$

$$S_{ij}^-=a_{i\downarrow}^\dagger a_{j\uparrow}, \quad (3)$$

where $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) creates (destroys) an electron with spin σ at site i. Using $S_{ij}^\pm$, one may define a generalized susceptibility

$$\chi_{ijkl}^{+-}(t)=\langle\langle S_{ij}^+(t);S_{kl}^-(0)\rangle\rangle. \quad (4)$$

Clearly, the transverse spin susceptibility we wish to calculate is $\chi_{ij}^{+-}(t)=\chi_{iijj}^{+-}(t)$. In order to calculate it, we consider that the electronic structure of the system is described by a simple one-band Hubbard Hamiltonian

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^\dagger a_{j\sigma}+\sum_{i\sigma}\epsilon_i n_{i\sigma}+\sum_i U_i n_{i\uparrow}n_{i\downarrow}, \quad (5)$$

where t_{ij} is the hopping integral between sites i and j ($t_{ii}=0$), ϵ_i is an atomic energy level, U_i represents the effective Coulomb interaction between two electrons on the same site i, and $n_{i\sigma}=a_{i\sigma}^\dagger a_{i\sigma}$ is the corresponding electronic occupation number.

In this case, $\chi_{ijkl}^{+-}(t)$ obeys the following equation of motion:

$$\begin{aligned} i\hbar\frac{d\chi_{ijkl}^{+-}(t)}{dt}&=\delta(t)\langle a_{i\uparrow}^\dagger a_{l\uparrow}\delta_{jk}-a_{k\downarrow}^\dagger a_{j\downarrow}\delta_{il}\rangle \\ &+\sum_n [t_{jn}\chi_{inkl}^{+-}(t)-t_{ni}\chi_{njkl}^{+-}(t)] \\ &+U_j\langle\langle[a_{i\uparrow}^\dagger a_{j\downarrow}a_{j\uparrow}^\dagger a_{j\uparrow}](t);S_{kl}^-(0)\rangle\rangle \\ &+U_i\langle\langle[a_{i\downarrow}^\dagger a_{i\downarrow}a_{i\uparrow}^\dagger a_{j\downarrow}](t);S_{kl}^-(0)\rangle\rangle. \end{aligned} \quad (6)$$

The appearance of higher-order Green's functions leads to an infinite chain of coupled equations for $\chi_{ijkl}^{+-}(t)$ that can be decoupled using the RPA, which consists of replacing

$$\begin{aligned} a_{i\sigma}^\dagger a_{j\sigma'}a_{k\xi}^\dagger a_{l\xi'}\approx&\langle a_{i\sigma}^\dagger a_{j\sigma'}\rangle a_{k\xi}^\dagger a_{l\xi'}-\langle a_{i\sigma}^\dagger a_{l\xi'}\rangle a_{k\xi}^\dagger a_{j\sigma'} \\ &+\langle a_{k\xi}^\dagger a_{l\xi'}\rangle a_{i\sigma}^\dagger a_{j\sigma'}-\langle a_{k\xi}^\dagger a_{j\sigma'}\rangle a_{i\sigma}^\dagger a_{l\xi'}. \end{aligned} \quad (7)$$

Here, the expectation values are evaluated in the Hartree-Fock ground state, where the dynamics of the two spin projections are treated independently. As a result, the average of products of two operators associated with opposite spins vanishes. Therefore, one obtains

$$\begin{aligned} i\hbar\frac{d\chi_{ijkl}^{+-}(t)}{dt}&=\delta(t)\langle a_{i\uparrow}^\dagger a_{l\uparrow}\delta_{jk}-a_{k\downarrow}^\dagger a_{j\downarrow}\delta_{il}\rangle \\ &+\sum_{m,n}(\delta_{im}t_{jn}-\delta_{jn}t_{mi})\chi_{mnkl}^{+-}(t) \\ &+\sum_{m,n}\delta_{mn}U_m(\delta_{im}\langle a_{i\downarrow}^\dagger a_{j\downarrow}\rangle \\ &-\delta_{jm}\langle a_{i\uparrow}^\dagger a_{j\downarrow}\rangle)\chi_{mnkl}^{+-}(t). \end{aligned} \quad (8)$$

The Fourier transform of Eq. (8) then reads

$$\begin{aligned} \hbar\omega\chi_{ijkl}^{+-}(\omega)=D_{ijkl}+\sum_{mn}&[K_{ijmn}\chi_{mnkl}^{+-}(\omega)+J'_{ijmn}\chi_{mnkl}^{+-}(\omega) \\ &+J_{ijmn}\chi_{mnkl}^{+-}(\omega)], \end{aligned} \quad (9)$$

where $\hat{D}$, $\hat{K}$, $\hat{J}'$, and $\hat{J}$ are four-indices matrices defined by

$$D_{ijkl}=\langle a_{i\uparrow}^\dagger a_{l\uparrow}\delta_{jk}-a_{k\downarrow}^\dagger a_{k\downarrow}\delta_{il}\rangle,$$

$$K_{ijkl}=\delta_{ik}t_{jl}-\delta_{jl}t_{ki},$$

$$J_{ijkl}=\delta_{kl}U_k(\delta_{ik}\langle a_{i\downarrow}^\dagger a_{j\downarrow}\rangle-\delta_{jk}\langle a_{i\uparrow}^\dagger a_{j\uparrow}\rangle),$$

$$J'_{ijkl}=\delta_{ik}\delta_{jl}(U_j\langle n_{j\uparrow}\rangle-U_i\langle n_{i\downarrow}\rangle). \quad (10)$$

The matrix elements of the product of two of such matrices is given by $(\hat{A}\hat{B})_{ijkl}=\Sigma_{mn}A_{ijmn}B_{mnkl}$. Thus, we may rewrite Eq. (9) in matrix form as

$$\hbar\omega\hat{\chi}^{+-}(\omega)=\hat{D}+(\hat{K}+\hat{J}+\hat{J}')\hat{\chi}^{+-}(\omega). \quad (11)$$

This equation may be also rewritten as

$$\hat{\chi}^{+-}(\omega)=\hat{\chi}^{\mathrm{HF}}(\omega)+\hat{\chi}^{\mathrm{HF}}(\omega)\hat{P}\hat{\chi}^{+-}(\omega), \quad (12)$$

where $\hat{P}=\hat{D}^{-1}\hat{J}$, and $\hat{\chi}^{\mathrm{HF}}(\omega)$ represents the susceptibility $\hat{\chi}^{+-}(\omega)$ calculated within one-electron theory, i.e., in the Hartree-Fock (HF) approximation. $\hat{\chi}^{\mathrm{HF}}(\omega)$ satisfies the following equation:

$$\hbar\omega\hat{\chi}^{\mathrm{HF}}(\omega)=\hat{D}+(\hat{K}+\hat{J}')\hat{\chi}^{\mathrm{HF}}(\omega). \tag{13}$$

Therefore, by using Eq. (10) we find

$$\chi_{ijkl}^{+-}(\omega)=\chi_{ijkl}^{\mathrm{HF}}(\omega)-\sum_m \chi_{ijmm}^{\mathrm{HF}}(\omega)U_m\chi_{mmkl}^{+-}(\omega). \tag{14}$$

The dynamic susceptibility $\chi_{ij}^{+-}(t)=\chi_{iijj}^{+-}(t)$ is then given by

$$\chi_{ij}^{+-}(\omega)=\chi_{ij}^{\mathrm{HF}}(\omega)-\sum_m \chi_{im}^{\mathrm{HF}}(\omega)U_m\chi_{mj}^{+-}(\omega). \tag{15}$$

In the HF approximation, $\uparrow$- and $\downarrow$-spin electrons are independent, and an electron with spin σ at site i is subjected to the HF potential

$$\epsilon_{i\sigma}=\epsilon_i+U_i\langle n_{i-\sigma}\rangle. \tag{16}$$

It follows that $\chi_{ij}^{\mathrm{HF}}(\omega)$ can be expressed in terms of the HF one-electron propagators as

$$\chi_{ij}^{\mathrm{HF}}(\omega)=-\langle a_{i\uparrow}^{\dagger}(t)a_{j\uparrow}\rangle G_{ij}^{\downarrow}(t)+\langle a_{j\downarrow}^{\dagger}a_{i\downarrow}(t)\rangle G_{ij}^{\uparrow *}(t), \tag{17}$$

where $G_{ij}^{\sigma}(t)$ is the time-dependent one-particle retarded Green's function for electrons with spin σ, connecting sites i and j, defined by

$$G_{ij}^{\sigma}(t)=-\frac{i}{\hbar}\Theta(t)\langle\{a_{i\sigma}(t),a_{j\sigma}^{\dagger}\}\rangle, \tag{18}$$

where the braces denote an anticommutator. The correlation functions in Eq. (17) can be written in terms of the one-particle Green's functions as

$$\langle a_{i\sigma}^{\dagger}(t)a_{j\sigma}\rangle=\frac{1}{\pi}\int d\omega\, f(\omega)\,\mathrm{Im}\,G_{ji}^{\sigma}(\omega)e^{i\omega t},$$

$$\langle a_{j\sigma}^{\dagger}a_{i\sigma}(t)\rangle=-\frac{1}{\pi}\int d\omega\, f(\omega)\,\mathrm{Im}\,G_{ij}^{\sigma}(\omega)e^{-i\omega t}, \tag{19}$$

where

$$\mathrm{Im}\,G_{ij}^{\sigma}(\omega)=\frac{1}{2i}[G_{ij}^{\sigma}(\omega)-G_{ji}^{\sigma *}(\omega)]. \tag{20}$$

After Fourier transforming Eq. (17) and using Eq. (19) one obtains

$$\chi_{ij}^{\mathrm{HF}}(\omega)=-\frac{1}{\pi}\int d\omega'\, f(\omega')[\mathrm{Im}\,G_{ji}^{\uparrow}(\omega')G_{ij}^{\downarrow}(\omega'+\omega)$$
$$+\mathrm{Im}\,G_{ij}^{\downarrow}(\omega')G_{ji}^{\uparrow -}(\omega'-\omega)], \tag{21}$$

where $G_{ji}^{\sigma -}(\omega)$ is the advanced one-particle Green's function.

Since we are interested in multilayer structures having translational symmetry parallel to the layers, it is convenient to work with a mixed representation by choosing our basis as Bloch sums in a single atomic plane l defined by

$$\phi_l(\mathbf{q}_\parallel)=\frac{1}{N_\parallel}\sum_{j\in l}\varphi(\mathbf{R}_j)e^{i\mathbf{q}_\parallel\cdot\mathbf{R}_j}. \tag{22}$$

Here $\varphi(\mathbf{R}_j)$ denotes an atomic orbital centered at site $\mathbf{R}_j \in l$, $\mathbf{q}_\parallel$ is a wave vector parallel to the layers, and $N_\parallel$ is the number of sites in this plane. Owing to the fact that $\mathbf{q}_\parallel$ is a good quantum number, the Hartree-Fock susceptibility in such a representation is given by

$$\chi_{ll'}^{\mathrm{HF}}(\mathbf{q}_\parallel,\omega)=-\frac{1}{\pi}\int d\omega'\, f(\omega')\frac{1}{N_\parallel}$$
$$\times\sum_{\mathbf{k}_\parallel}[\mathrm{Im}\,G_{l'l}^{\uparrow}(\mathbf{k}_\parallel,\omega')G_{ll'}^{\downarrow}(\mathbf{q}_\parallel+\mathbf{k}_\parallel,\omega'+\omega)$$
$$+\mathrm{Im}\,G_{ll'}^{\downarrow}(\mathbf{k}_\parallel,\omega')G_{l'l}^{\uparrow -}(\mathbf{k}_\parallel-\mathbf{q}_\parallel,\omega'-\omega)]. \tag{23}$$

Similarly to Eq. (15), the in-plane dynamic susceptibility satisfies the following equation:

$$\chi_{ll}^{+-}(\mathbf{q}_\parallel,\omega)=\chi_{ll}^{\mathrm{HF}}(\mathbf{q}_\parallel,\omega)-\sum_m \chi_{lm}^{\mathrm{HF}}(\mathbf{q}_\parallel,\omega)U_m\chi_{ml}^{+-}(\mathbf{q}_\parallel,\omega). \tag{24}$$

It is noteworthy that Eq. (24) couples the susceptibility matrix elements involving atomic planes with $U\neq 0$ only. Thus, for a magnetic film of finite thickness on a noninteracting substrate, the set of Eq. (24) can be solved in matrix form as

$$\chi^{+-}(\mathbf{q}_\parallel,\omega)=[I+\chi^{\mathrm{HF}}(\mathbf{q}_\parallel,\omega)U]^{-1}\chi^{\mathrm{HF}}(\mathbf{q}_\parallel,\omega), \tag{25}$$

where $[I+\chi^{\mathrm{HF}}U]$ is a matrix in plane indices having finite dimension equal to the number of atomic planes of the magnetic film.

III. SPIN WAVES IN SOME OVERLAYERS

Within a single-band tight-binding model it would be pretentious to expect an accurate quantitative description of real magnetic systems. Nevertheless, such a simple model contains the necessary physical ingredients for a good qualitative analysis of the main electronic properties and characteristics of metallic systems in general. Given the modelistic nature of our calculation, we have selected representative parameters, rather than attempting to adjust them to fit a very specific system.

We consider a monolayer of a metallic ferromagnet on a surface of a nonmagnetic semi-infinite metallic substrate. The systems we have in mind are made up of transition metals. Their electronic structures are described by the Hamiltonian given by Eq. (5). In this case, our single orbital represents a set of d orbitals. We take into account hopping between nearest-neighbor sites only, and assume that it is the same ($t_{ij}=t$) both in the substrate and in the overlayer. This

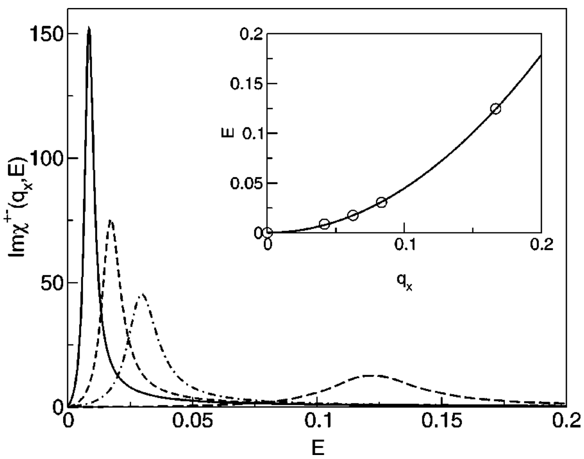

FIG. 1. Spin-wave spectrum for the (100) overlayer. The figure shows Im $\chi^{+-}(\mathbf{q}_{\parallel},\omega)$ calculated as a function of energy $E=\hbar\omega$ for several values of $\mathbf{q}_{\parallel}=q_x\hat{x}$ along the [100] direction. Solid line is for $q_x=0.042$, dashed line for $q_x=0.063$, dot-dashed line for $q_x=0.083$, and long-dashed line for $q_x=0.166$. All values of q_x are in units of $2\pi/a$, where a is the lattice constant. The inset show the corresponding spin-wave energies obtained from the positions of the peaks of Im χ^{+-}.

is a reasonable assumption for transition metals belonging to the same row of the periodic table. We examine overlayers placed on (100) and (110) surfaces of a simple cubic lattice. One may argue that transition metals do not crystallize in simple cubic lattices, but this is not essential for the type of effects we wish to address. With the intention to simulate a nonmagnetic substrate having a relatively large number of holes, we set the atomic energy levels ϵ_i and the effective on-site Coulomb interactions U_i both equal to zero in the substrate, and fix the Fermi energy at $E_F=0.15$. Here all energies are measured in units of the nearest-neighbor hopping t. Such a choice of parameters gives a bulk substrate occupancy $n=1.06$ e/at, and is appropriate for nonmagnetic transition metals with approximately half-filled d bands. In order to describe a monolayer of a strong ferromagnet built atop the substrate, we take $U_i=12$ in the surface layer and determine the surface-atomic energy level ϵ_s (assuming a common value of E_F) so that the overlayer has an electronic occupancy $n_s=1.68$ e/at (suitable for Co in this single-band model). The HF ferromagnetic ground state of the system is then calculated self-consistently. A relatively large value of U in the overlayer was chosen to guarantee a stable ferromagnetic HF ground state with a number of holes in the majority-spin band of the overlayer much smaller than in the minority one. The spin-wave spectrum is obtained by calculating the surface transverse spin susceptibility $\chi^{+-}(\mathbf{q}_{\parallel},\omega)$, using Eqs. (25) and (23).

First we study a ferromagnetic monolayer on a (100) surface. Figure 1 shows Im $\chi^{+-}(\mathbf{q}_{\parallel},\omega)$ calculated as a function of energy $E=\hbar\omega$ for several values of $\mathbf{q}_{\parallel}$ along the [100] direction in the surface plane. The lifetime of a spin wave with wave vector $\mathbf{q}_{\parallel}$ is inversely proportional to the width of the peak of Im $\chi^{+-}(\mathbf{q}_{\parallel},\omega)$. Such width may be influenced by the small imaginary part η usually added to the energy in

TABLE I. Magnetic moments of the surface layer (in units of the Bohr magneton) calculated for different values of the hopping $t_{\perp}=\alpha t$ between the substrate and the overlayer. Except for $\alpha=0$ all values of m_s have been determined self-consistently.

α	1.0	0.8	0.6	0.3	0.1	0.0
m_s	0.275	0.292	0.304	0.316	0.320	0.320

numerical calculations of $\chi^{+-}(\mathbf{q},\omega)$. Our calculations for the [100] direction were all made with the value of $\eta=1\times10^{-2}$, and for the [110] direction we have used $\eta=5\times10^{-3}$ for numerical convergence reasons. It is clear from Fig. 1 that the spin waves in the overlayer become strongly damped for increasing values of $q_{\parallel}$. The spin-wave energies $E(\mathbf{q}_{\parallel})$ were obtained from the position of the peak in Im $\chi^{+-}(\mathbf{q}_{\parallel},\omega)$. The inset in Fig. 1 shows that E varies quadratically with $q_{\parallel}$ over a wide range of values in the first Brillouin zone.

The explanation for the spin-wave damping in the overlayer, given in Ref. 12, is based on the tunneling of holes from the nonmagnetic substrate into the majority-spin band of the overlayer. Without a substrate, the free-standing ferromagnetic monolayer would have a well-defined Stoner gap, and the spin waves infinitely long lifetimes. The tunneling of holes from the substrate into the overlayer destroys this well-defined Stoner gap allowing the spin waves to decay into electron-hole pairs. To prove that such an explanation is correct we have gradually disconnected the overlayer from the substrate by artificially reducing the hopping $t_{\perp}=\alpha t$ between the surface layer and the substrate. We consider several values of $0\leqslant\alpha\leqslant1$, recalculating in each case the HF ground state self-consistently. The corresponding values of the surface layer magnetic moments are listed in Table I. As expected, the ground state magnetic moment slightly increases as α decreases. Figure 2 shows Im $\chi^{-+}(E,q_{\parallel})$, cal-

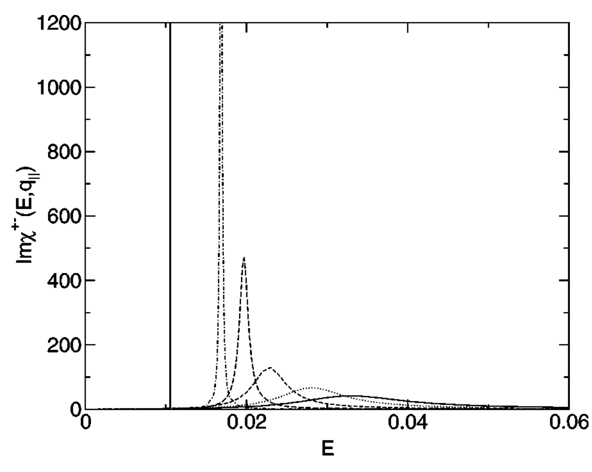

FIG. 2. Im $\chi^{-+}(q_{\parallel},E)$ calculated as a function of $E=\hbar\omega$ for a fixed $q_{\parallel}=0.083$ along the [100] direction, and different values of the hopping $t_{\perp}=\alpha t$ between the (100) surface layer and the substrate. Thin-solid line is for $\alpha=1.0$, dotted line for $\alpha=0.8$, dashed line for $\alpha=0.6$, long-dashed line for $\alpha=0.3$, dot-dashed line for $\alpha=0.1$, and thick-solid line for $\alpha=0$.

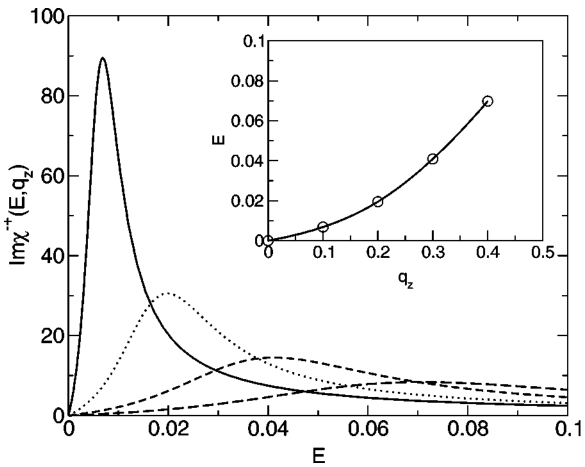

FIG. 3. Spin-wave spectrum for the (110) overlayer. The figure shows $\mathrm{Im}\,\chi^{+-}(\mathbf{q}_{\|},\omega)$ calculated as a function of energy $E=\hbar\omega$ for several values of $\mathbf{q}_{\|}=q_z\hat{z}$ along the [001] direction. Solid line is for $q_z=0.1$, dotted line for $q_z=0.2$, dashed line for $q_z=0.3$, and long-dashed line for $q_z=0.4$. All values of q_z are in units of $2\pi/a$, where a is the lattice constant. The inset shows the corresponding spin-wave energies obtained from the positions of the peaks of $\mathrm{Im}\,\chi^{+-}$.

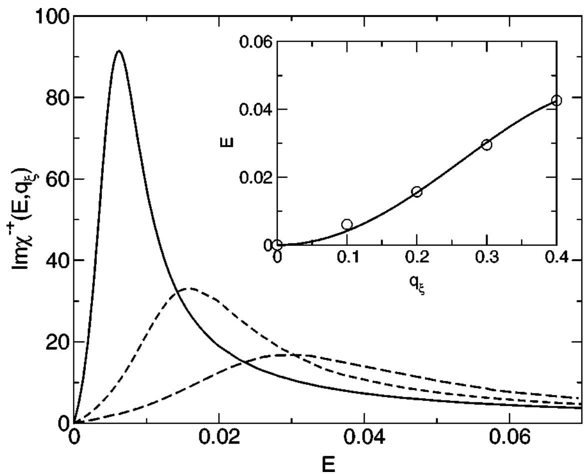

FIG. 4. Spin-wave spectrum for the (110) overlayer. The figure shows $\mathrm{Im}\,\chi^{+-}(\mathbf{q}_{\|},\omega)$ calculated as a function of energy $E=\hbar\omega$ for several values of $\mathbf{q}_{\|}=q_\xi\hat{\xi}$ along the $[1\bar{1}0]$ direction. Solid line is for $q_\xi=0.1$, dashed line for $q_\xi=0.2$, and long-dashed line for $q_\xi=0.3$. All values of q_ξ are in units of $2\pi/a$, where a is the lattice constant. The inset shows the corresponding spin-wave energies obtained from the positions of the peaks of $\mathrm{Im}\,\chi^{+-}$.

culated as a function of E for different values of α, and $q_{\|}=0.083\times 2\pi/a$, where a is the lattice constant. When α decreases, so does the tunneling of holes from the substrate into the overlayer. Thus, the decaying probability of the spin waves is reduced and their lifetimes increase. Consequently, the widths of the spin-wave peaks become narrower, as evidenced in Fig. 2. It is also noticeable from Fig. 2 that the spin-wave energies become smaller as α decreases. This is partially due to the reduction of the exchange coupling between the local moments, mediated by the substrate when α decreases. This shows that the presence of a nonmagnetic substrate may substantially affect the spin-wave spectrum of the monolayer.

We now examine a ferromagnetic monolayer on a (110) surface. Figures 3 and 4 show results of $\mathrm{Im}\,\chi^{+-}(\mathbf{q}_{\|},E)$, calculated as a function of energy for several values of $\mathbf{q}_{\|}$ along the [001] ($\hat{z}$) and $[1\bar{1}0]$ ($\hat{\xi}$) directions in the surface plane, respectively. The spin-wave energy for the (110) surface is not isotropic in $\mathbf{q}_{\|}$ space. The origin for such anisotropy lays on the crystalline structure of the (110) overlayer. For a simple cubic lattice it is formed by chains of nearest-neighbor sites along the $\hat{z}$ direction that, in the absence of second-neighbor hopping, are linked to each other via the substrate only. Thus, without a substrate [i.e., for a free-standing (110) monolayer], those chains would be uncoupled, and no energy would be required to excite long-wavelength spin waves propagating perpendicularly to the chains.[9] The inset in Fig. 3 shows that the dispersion relation for spin waves propagating along $\hat{z}$ varies quadratically with q_z over a wide range of values in the first Brillouin zone. In contrast, the inset of Fig. 4 shows that for $\mathbf{q}_{\|}$ perpendicular to the chains, $E(q_\xi)$ deviates from the quadratic behavior for relatively low values of q_ξ.

By comparing the insets of Figs. 3 and 4, we note that the energy of a spin wave propagating along $[1\bar{1}0]$ in the (110) overlayer is smaller than when it propagates along the $\hat{z}$ direction with the same $|\mathbf{q}_{\|}|$. The difference in energies, however, is not as large as previously found for unsupported monolayers.[9] The reason is the exchange interaction between the chains that is mediated by the substrate. Although smaller, it is comparable to the direct exchange interaction between nearest-neighbor sites along the chains, leading to a stiffness along $[1\bar{1}0]$, which is of the same order of magnitude as that along $\hat{z}$.

By reducing the hopping from the overlayer to the substrate, the interchain coupling decreases and the energy to

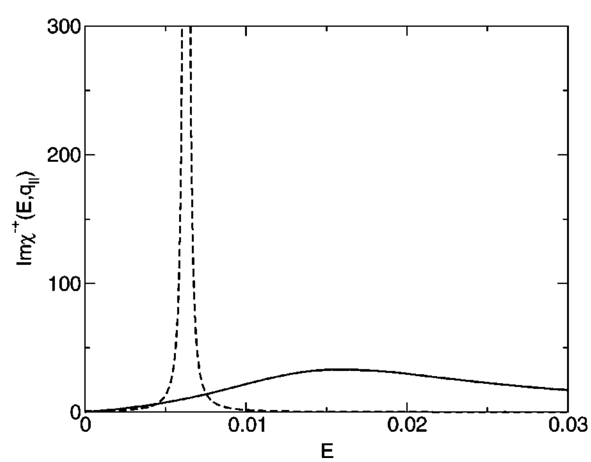

FIG. 5. $\mathrm{Im}\,\chi^{-+}(q_{\|},E)$ calculated as a function of $E=\hbar\omega$ for a fixed value of $\mathbf{q}_{\|}=0.2\hat{\xi}$, where $\hat{\xi}$ is a unit vector along the $[1\bar{1}0]$ direction in the (110) surface plane. The solid and dashed lines correspond to different values of the hopping $t_\perp=\alpha t$ between the (110) surface layer and the substrate. Solid line is for $\alpha=1.0$ and dashed line for $\alpha=0.1$.

excite a spin wave propagating along $[1\bar{1}0]$ becomes substantially smaller. This is illustrated in Fig. 5, and it is qualitatively in accordance with what has been found in Ref. 9.

IV. CONCLUSIONS

We have investigated the influence of a nonmagnetic metallic substrate on the spin excitations in ultrathin ferromagnetic overlayers. Both the spin-wave energies and lifetimes have been determined by calculating the transverse dynamic spin susceptibility $\chi^{+-}(\mathbf{q}_{\parallel},E)$ for different surface crystalline orientations. We have found that the spin waves in the overlayer are strongly damped due to the presence of the substrate. By gradually reducing the hopping between the substrate and the overlayer we were able to assess how much the substrate may affect the lifetimes and energies of spin waves excited in the overlayer. We have shown that the spin-wave lifetimes increase substantially as the hopping between the substrate and the overlayer decreases. This verifies that the spin-wave damping is caused by the tunneling of holes from the substrate into the overlayer, as previously pointed out by Phan *et al.*[12] We have also shown that the spin-wave energies may change considerably when the substrate-overlayer hopping is varied. The main reason for that is the alteration of the exchange coupling mediated by the substrate, a quantity that relies much on such hopping.

For the (110) overlayer we have found that the spin-wave energy depends upon the direction of the wave vector $\mathbf{q}_{\parallel}$ along which it is excited. Such dependence, however, is much less pronounced than previously obtained for unsupported monolayers. We argue that this is due to the enhancement of the exchange coupling between the local moments in the overlayer mediated by the substrate, which strongly affects the spin-wave energies.

We hope that our findings will stimulate more elaborate calculations for specific real systems. Perhaps, a gradual disconnection of the overlayer from the substrate may also be realized experimentally by placing nonmetallic spacer layers of variable thicknesses between the overlayer and the substrate, allowing the effects discussed here to be observed.

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