Breakdown of the adiabatic approach for magnetization damping in metallic ferromagnets

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We present a microscopic theory for magnetization relaxation in metallic ferromagnets of nanoscopic dimensions that is based on the calculation of the dynamic spin response matrix in the presence of spin-orbit coupling. Our approach takes into account the collective character of spin excitations in ferromagnetic metals. We show that calculations of the Gilbert damping based on a mean-field, adiabatic approximation fail to describe the relaxation of collective excitations in the ballistic regime. Namely, we show that collective spin excitations such as the ferromagnetic resonance mode have finite damping rates even for perfectly crystalline systems, whereas existing microscopic approaches, based on adiabatic and mean-field approximations, predict infinite damping rates. Moreover, we demonstrate that within a finite frequency approach the relaxation properties are not completely determined by the transverse susceptibility alone, and that the damping rate has a non-negligible frequency dependence in experimentally relevant situations. Our results indicate that the widely used adiabatic approach for spin dynamics breaks down for metallic nanostructures in the presence of strong spin-orbit coupling.

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Magnetization relaxation in metals is at the heart of spin current generation and detection processes currently under investigation, many of them candidates to play protagonist roles in innovative spintronic devices. The Landau-Lifshitz-Gilbert (LLG) equation is widely used to describe the spin dynamic properties of magnetic materials [1,2]. It includes an important system-dependent parameter, called the Gilbert damping parameter, usually denoted by α_G, that regulates the relaxation of the magnetization towards stability, after it is driven out of equilibrium. Recently, a lot of effort has been put into the determination of this damping rate [2–8], which characterizes the pumping and absorption of pure spin currents in nanostructures that are of great interest in the field of spintronic. In most of them spin-orbit interaction is significant, and responsible for a desirable interplay between charge spin and angular momentum excitations.

There is a general agreement between practitioners in the field that a proper microscopic theory of magnetization relaxation in metals requires a good description of the electronic structure of the system including spin-orbit coupling [3–8]. The conventional approach is to combine a realistic electronic structure with some kind of adiabatic approximation and, within a mean-field treatment of the magnetization dynamics, to derive expressions that can be directly related to the Landau-Lifshitz-Gilbert phenomenology. This strategy has been employed by Kamberský [3] and many others since [4–8]. This conventional approach has important limitations. First and foremost, it adopts the view that, in order to obtain the damping parameter of a system, it is enough to consider its mean-field transverse spin response. Furthermore, it assumes the linewidth of the zero wave vector spin wave resonance is completely determined by the zero frequency limit of the mean-field transverse susceptibility. In doing so, it neglects the coupling between transverse spin, longitudinal spin, and charge excitations (which is an important consequence of the spin-orbit coupling). It also incorrectly predicts the divergence of the damping parameter for a perfectly crystalline system at zero temperature. Actually, for ferromagnets that display rotation symmetry in spin space, the Goldstone theorem ensures that any experiment which measures the total transverse magnetic moment of the sample will produce a resonant response with zero linewidth [9]. Even in the presence of disorder the uniform mode should still have infinite lifetime, since this is a consequence of the invariance of the system's Hamiltonian to global rotations in spin space. In the presence of spin-orbit interaction, however, this symmetry is explicitly broken, and the resonant spectrum acquires a finite linewidth [10].

We put forward a more fundamental microscopic approach to the calculation of the spin dynamics damping rate that takes fully into account the effects of SOC on the spectrum of spin excitations of itinerant systems. Namely, by studying the magnetization dynamics within a ladder approximation treatment of the screened Coulomb repulsion, we naturally incorporate the coupling of transverse spin excitations to longitudinal spin and charge excitations, induced by the spin-orbit interaction [10]. We calculate the FMR spectrum at finite frequencies and arbitrary anisotropy values, without employing any adiabatic approximation. Thus, the main difference between our approach and previous approaches found in the literature is the fact that we treat the spin excitations as collective excitations, whereas the existing approaches describe the magnetization dynamics as a semiclassical motion of the magnetization due to a slow change of the mean exchange field. We will show that treating the spin dynamics as resulting from collective excitations is an essential ingredient to correctly describe the magnetization relaxation in very clean metallic ferromagnets of nanoscopic dimensions at low temperatures.

Our work is organized as follows: We will present briefly our formalism, discuss its main features, and present numerical results for two model systems that illustrate common but qualitatively different situations. We will also present a version of the adiabatic mean-field approach that allows us to compare the effects of those approximations to the predictions of our approach without abandoning completely our calculation scheme.

General formalism. The spectrum of spin excitations of a ferromagnet can be obtained from the spectral density associated with the transverse spin susceptibility,

$$\chi^{+-}(l,l';\Omega) = \int dt e^{i\Omega t} \langle\langle S_l^+(t), S_{l'}^-(0)\rangle\rangle, \quad (1)$$

where

$$\langle\langle S_l^+(t), S_{l'}^-(0)\rangle\rangle \equiv -i\theta(t)\langle[S_l^+(t), S_{l'}^-(0)]\rangle, \quad (2)$$

and

$$S_l^+ = \sum_\mu a_{l\mu\uparrow}^\dagger a_{l\mu\downarrow}. \quad (3)$$

The operator $a_{l\mu\sigma}^\dagger$ creates one electron in the atomic basis state μ localized at lattice site l with spin σ. Here Ω represents the frequency of the applied transverse magnetic field, and $\theta(t)$ is the usual step function which is equal to unit for $t > 0$ and zero otherwise. Although we are usually interested in $\chi^{+-}(l,l';\Omega)$ as defined above, its equation of motion involves the orbital-resolved susceptibility,

$$\chi^{+-}_{\mu\nu\mu'\nu'}(l,l';t) \equiv \langle\langle a_{l\mu\uparrow}^\dagger(t) a_{l\nu\downarrow}(t), a_{l'\mu'\downarrow}^\dagger(0) a_{l'\nu'\uparrow}(0)\rangle\rangle. \quad (4)$$

One notices that this susceptibility is actually a two-particle Green function, that describes the propagation of an electron and a hole of opposite spins. Within the mean-field approximation the electron and the hole propagate independently and this propagator describes what is known as Stoner excitations. In order to describe spin waves it is necessary at least to take into account the Coulomb interaction between the electron and the hole. The simplest approximation that incorporates this interaction is a partial summation of Feynman diagrams of the ladder type, sometimes also called a random phase approximation (RPA) [11]. In our treatment this interaction is brought about by a screened exchange term that acts among electrons occupying d orbitals within the same atomic site [10]. The ferromagnetic resonance mode, most relevant to the discussion of Gilbert damping, is actually the zero wave-vector limit of the spin wave mode.

In the absence of spin-orbit coupling (SOC) and within the RPA, the equation of motion for $\chi^{+-}_{\mu\nu\mu'\nu'}(l,l';t)$ is closed and $\chi^{+-}(l,l';\Omega)$ can be expressed in the well-known form,

$$\chi^{+-}(\Omega) = [1 + U\chi_0^{+-}(\Omega)]^{-1}\chi_0^{+-}(\Omega), \quad (5)$$

where $\chi_0^{+-}(\Omega)$ is the mean-field susceptibility. This expression is schematic and must be understood as a matrix in orbital and site indices, in real space, or a wave-vector-dependent matrix in reciprocal space. The crucial point, however, is that, in the absence of spin-orbit coupling, within the RPA, transverse spin excitations are decoupled from either longitudinal spin excitations or charge excitations. This ceases to be true when SOC is included, as we demonstrated in Ref. [10]: χ^{+-} becomes coupled to three other susceptibilities, namely

$$\chi^{(2)}_{\mu\nu\mu'\nu'}(l,l';t) \equiv \langle\langle a_{l\mu\uparrow}^\dagger(t) a_{l\nu\uparrow}(t), a_{l'\mu'\uparrow}^\dagger(0) a_{l'\nu'\uparrow}(0)\rangle\rangle, \quad (6)$$

$$\chi^{(3)}_{\mu\nu\mu'\nu'}(l,l';t) \equiv \langle\langle a_{l\mu\downarrow}^\dagger(t) a_{l\nu\downarrow}(t), a_{l'\mu'\downarrow}^\dagger(0) a_{l'\nu'\downarrow}(0)\rangle\rangle, \quad (7)$$

$$\chi^{(4)}_{\mu\nu\mu'\nu'}(l,l';t) \equiv \langle\langle a_{l\mu\downarrow}^\dagger(t) a_{l\nu\uparrow}(t), a_{l'\mu'\uparrow}^\dagger(0) a_{l'\nu'\downarrow}(0)\rangle\rangle. \quad (8)$$

The system of equations of motion obeyed by these four susceptibilities can be cast into a form strongly resembling the RPA result by introducing a block vector $\vec{\chi} \equiv (\chi^{(1)}, \chi^{(2)}, \chi^{(3)}, \chi^{(4)})^T$, with $\chi^{(1)} \equiv \chi^{+-}$. With an equivalent definition for the mean-field susceptibilities $\chi_0^{(m)}$ we write

$$\vec{\chi}(\Omega) = \vec{\chi}_0(\Omega) - \Lambda\vec{\chi}(\Omega), \quad (9)$$

where the "super-matrix" Λ is proportional to the effective Coulomb interaction strength and involves convolutions of single particle Green functions. Explicit forms for its matrix elements are found in Ref. [10]. The numerical analysis of the susceptibilities $\chi^{(2)}$, $\chi^{(3)}$, and $\chi^{(4)}$ show that their absolute values are many orders of magnitude smaller than those of $\chi^{(1)} = \chi^{+-}$. It is, thus, tempting to argue that the transverse susceptibility is approximately decoupled from $\chi^{(2)}$, $\chi^{(3)}$, and $\chi^{(4)}$ and that it can be calculated via the usual RPA expression with the single particle Green functions obtained with spin-orbit coupling taken into account. This is not a good approximation in general, since the matrix elements of Λ that couple $\chi^{(1)}$ to the other susceptibilities are far from negligible. Our numerical calculations indicate that they are essential to determine correctly the features of the FMR mode around the resonance frequency. Thus, the behavior of $\chi^{(1)}$ in the presence of spin-orbit coupling cannot be inferred from $\chi_0^{(1)}$ in the zero-frequency limit alone, as it is usually assumed in the literature on the calculation of the Gilbert damping parameter [3–5,8,12].

Numerical results. We start the discussion by presenting results for the Gilbert parameter α_G for unsupported ultrathin Co films. We define α_G as the ratio between the FMR linewidth $\Delta\Omega$ and the resonance frequency Ω_0. First we turn off spin-orbit coupling to check the consistency of our approach. Even with SOC turned off we still find a finite linewidth for the FMR mode. It comes, as we will shortly demonstrate, from the small imaginary part η that is usually added to the energy in the numerical calculations of the single particle Green functions, in order to shift their poles from the real axis. We calculate α_G for various values of η and extrapolate to $\eta \to 0^+$, as shown in Fig. 1. It is clear that

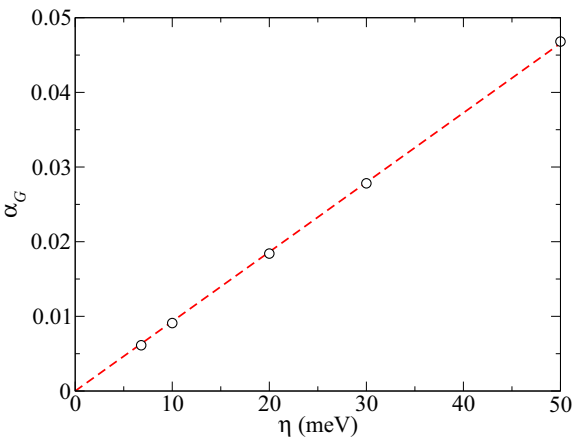

FIG. 1. (Color online) Gilbert damping parameter α_G as a function of the imaginary part η added to the real energy, for an ultrathin film of two atomic layers of Co where SOC has been turned off. It is clear that α_G vanishes as $\eta \to 0$.

$\lim_{\eta\to 0^+}\alpha_G = 0$. Thus, our approach correctly predicts that the Gilbert damping parameter vanishes in the absence of SOC, as it should. Indeed, it is easy to show [9] that the FMR mode is a stationary state of the mean-field Hamiltonian and, as such, has infinite lifetime in the limit $\eta \to 0^+$. Now we discuss the dependence of α_G on η for a fixed, nonzero value of the spin-orbit coupling strength ξ. We used LCAO parameters appropriate for bulk Co to describe the electronic structure of all Co films we investigated. The quantitative details of the ferromagnetic ground state and excitation spectra are sensitive to the LCAO parameters used, but their qualitative behavior is very robust to small changes in the electronic structure. Our strategy is to use the same set of LCAO parameters for all film thicknesses to avoid modifications in α_G coming directly from changes in the LCAO parameters. This allows us to focus on geometric effects and on the η dependence.

Figure 2 shows the dependence of the Gilbert damping parameter α_G on the imaginary part η for Co films of various thicknesses. Clearly α_G approaches finite values as $\eta \to 0$. This is in sharp contrast with most approaches found in the literature, for which α_G is expected to diverge in the $\eta \to 0$ limit. In practice this would mean that the FMR mode should be so strongly damped in very clean samples at low temperatures that it would be very difficult to observe. To the best of our knowledge there are no signs of this divergent behavior in experimental results performed at low temperatures and high quality crystalline samples.

As we mentioned in the introduction, all existing approaches for calculating the Gilbert damping from the electronic structure are based on the evaluation of the transverse spin susceptibility within the mean-field approximation, in the limit of vanishing frequency [13]. We can apply both approximations to our approach, and also neglect the coupling of the transverse excitations to the longitudinal and charge excitations. This provides a direct assessment of the effect of those approximations without drifting too far away from our own approach. In Fig. 3 we show the comparison between the damping parameters obtained within the finite-frequency RPA and the adiabatic mean-field approaches for an unsupported Co monolayer. Besides the non-negligible quantitative discrepancy there is also a qualitatively different behavior as η decreases; the adiabatic mean-field α_G^{MFAd} seems to reach a minimum and starts to increase, whereas the nonadiabatic RPA α_G^{RPA} continues to decrease monotonically. Still in Fig. 3 we show the effect of increasing artificially the strength of SOC in Co. The discrepancy is clearly much bigger, both quantitatively and qualitatively.

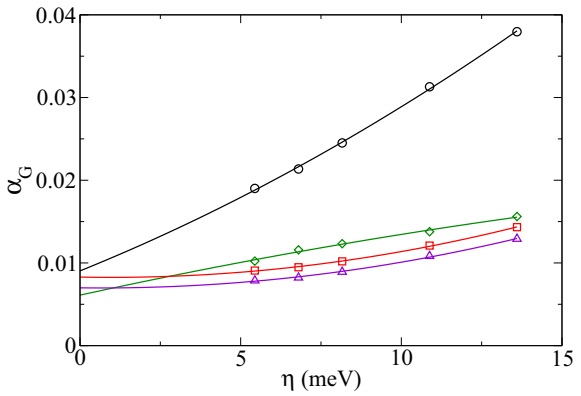

FIG. 2. (Color online) Gilbert damping parameter α_G as a function of the imaginary part η added to the energy, for Co ultrathin films of various thicknesses: one (circles), two (squares), four (diamonds), and six (triangles) atomic layers. The strength of the SOC is $\xi = 85$ meV. The solid lines are guides to the eye.

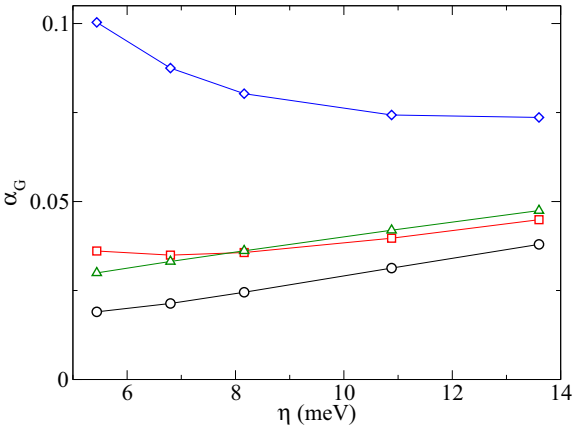

FIG. 3. (Color online) Gilbert damping parameter α_G calculated within the nonadiabatic RPA approach (black circles and green triangles), and within the adiabatic mean-field approximation (red squares and blue diamonds). The calculations are for a single Co atomic layer with $\xi_{\mathrm{Co}} = 85$ meV (black circles and red squares) and $\xi_{\mathrm{Co}} = 128$ meV (green triangles and blue diamonds).

Cobalt has a small spin-orbit coupling constant. We would like to investigate the effect of a large SOC strength on the damping rate in a more realistic setting than just tuning the SOC strength of Co. This can be achieved by considering layers of Co attached to a nonmagnetic substrate with high SOC parameter and partially filled d bands, such as Pt. This system has a particularly interesting feature: The magnetization easy axis is perpendicular to the plane. However, we found that, for the LCAO parameters we employed, the magnetization in-plane is also a stable configuration, with a small magnetocrystalline anisotropy. The damping rate, however, is much larger in the 2Co/2Pt system than in the unsupported Co films. This is a nice example of how the anisotropy energy is strongly influenced by the system's symmetry, but the damping rate is relatively insensitive to it, depending strongly on the intensity of the spin-orbit coupling. It is also an extremely convenient situation to test an assumption very frequently found in the literature on Gilbert damping, although sometimes not explicitly stated, that the FMR linewidth $\Delta\Omega$ is linearly dependent on the resonance frequency Ω_0 and that $\Delta\Omega \to 0$ as $\Omega_0 \to 0$. This is not an unreasonable hypothesis, considering the weak static fields commonly used in FMR experiments and the smallness of the spin-orbit coupling constant, compared to other energy scales of a ferromagnet. Our calculations for unsupported Co films confirm that this relationship approximately holds. In this case, the Gilbert parameter α_G may be extracted from the FMR spectrum obtained by sweeping either the Zeeman field or excitation frequency, and is practically independent of field or frequency. However, our results for 2Co/2Pt indicate that

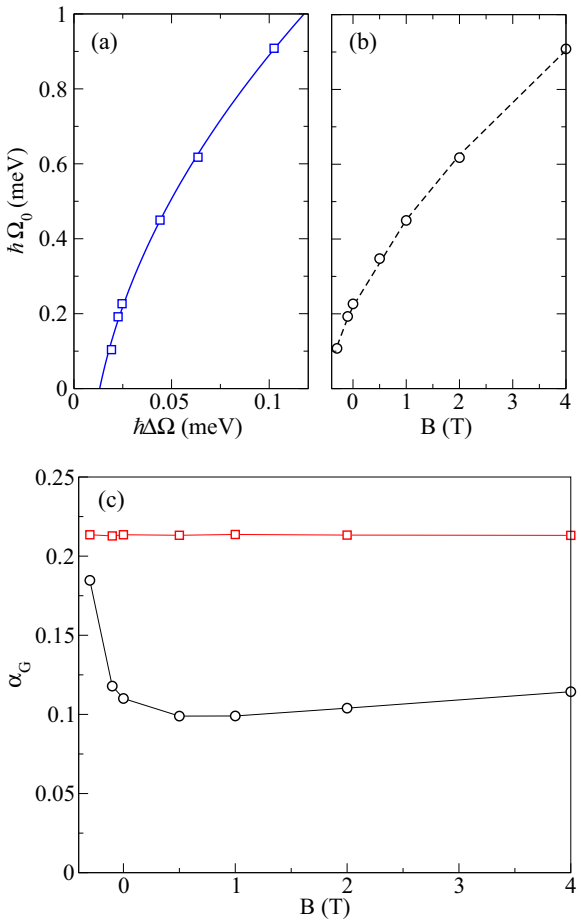

FIG. 4. (Color online) FMR frequency Ω_0 for the 2Co/2Pt system plotted as a function of FMR linewidths $\Delta\Omega$ (a), and as a function of the Zeeman field B (b). In (c) we show the Gilbert damping parameter α_G as a function of the applied Zeeman field B calculated with our nonadiabatic RPA approach (black circles) and the results for the adiabatic mean-field approximation (red squares). The strengths of the SOC are $\xi_{Co} = 85$ meV and $\xi_{Pt} = 600$ meV.

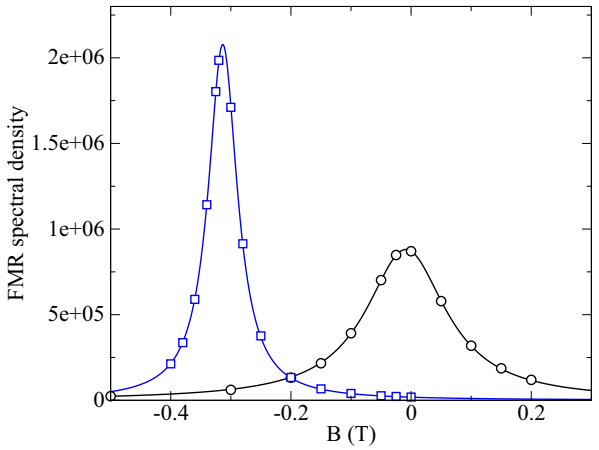

FIG. 5. (Color online) Spectral densities of the FMR mode for the 2Co/2Pt system plotted as a function of the Zeeman field B at fixed exciting frequencies: $\nu_p = 24$ GHz (squares) and $\nu_p = 54$ GHz (circles). The solid curves are Lorentzian fits to the calculated points.

the FMR linewidth approaches a finite value as $\Omega_0 \to 0$, as seen in Fig. 4(a). The corresponding resonance frequencies as a function of the Zeeman field may be seen in Fig. 4(b). This leads to a significantly frequency-dependent α_G, as shown in Fig. 4(c). Thus, it is impossible to characterize the damping rate of such a system by a single parameter. It is necessary either to consider the FMR linewidth explicitly as a function of frequency or to define a frequency-dependent damping parameter $\alpha_G(\Omega_0)$.

This discussion is also relevant for the interpretation usually employed to extract damping parameters from measured FMR spectra. In experiments the spectra are usually obtained as a function of Zeeman field intensity, for a fixed frequency of the exciting field. If the Gilbert parameter α_G were independent of frequency then the relationship between frequency sweeping and Zeeman field sweeping spectra would be straightforward. With α_G frequency dependent, however, the relationship is not trivial. In Fig. 5 we illustrate this issue by plotting the FMR spectral density as a function of the Zeeman field for two fixed exciting frequencies, 24 GHz and 54 GHz. The curves have nice Lorentzian shapes, but the values for the Gilbert damping parameter α_G extracted from these curves depend on the exciting frequency ($\alpha_G = 0.034$ for $\Omega_0 = 0.10$ meV and $\alpha_G = 0.042$ for $\Omega_0 = 0.22$ meV). Also, they do not correspond to any of the values shown in Fig. 4(c), although the Zeeman field values that determine the linewidth in Fig. 5 lie within the range of Zeeman field values shown in Fig. 4(b). Thus, with α_G defined as $\Delta\Omega/\Omega_0$, its value for a given sample depends on wether the FMR spectrum is obtained in a fixed frequency or fixed Zeeman field setup. Our results also imply that the existing expressions for the damping parameter α_G are not valid in general, especially for very clean systems with large spin-orbit coupling. The conventional approaches express α_G as the ratio $\Delta\Omega/\Omega_0$ in the $\Omega_0 \to 0$ limit. As we have just shown, this limit may not exist in some cases, since $\Delta\Omega$ approaches a finite value as $\Omega_0 \to 0$.

Once again we can compare our nonadiabatic RPA results with those obtained from an adiabatic mean-field approximation. In Fig. 4(c) we compare α_G^{MFAd} and α_G^{RPA} for the 2Co/2Pt system as a function of the applied Zeeman field. As expected, the mean-field adiabatic approximation predicts an essentially constant damping parameter, whereas the nonadiabatic RPA approach shows a large variation with the Zeeman field.

In experimental papers [14,15] the FMR linewidth is assumed to have a zero-frequency offset, just as we described. This is usually attributed to extrinsic broadening mechanisms, such as two-magnon scattering [16], due to the combination between inhomogeneities in the magnetic films and dipolar interactions. This is certainly the case in systems with small SOC, such as Fe films deposited on GaAs or Au [14]. However, we have shown that there can be zero-frequency offset of intrinsic origin if the SOC is large. The effect of this intrinsic offset should be easily separated from that of the two-magnon scattering mechanism, since the latter is not active when the magnetization is perpendicular to the plane of the film [16].

We would like to remark that Stoner enhancement in Pt also plays a very important role in the determination of the damping rate. We had shown previously [17] that, in the absence of spin-orbit coupling, Stoner enhancement had a very mild

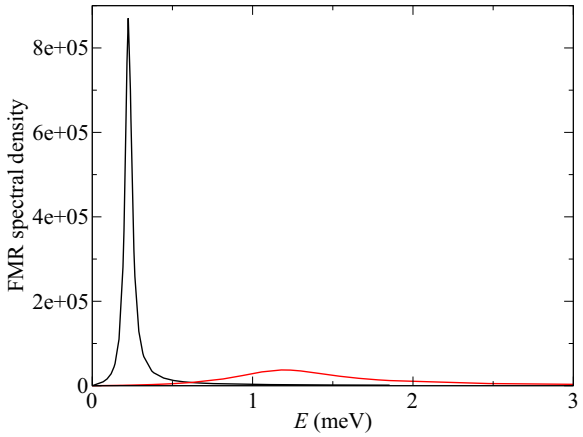

FIG. 6. (Color online) Spectral densities of the FMR mode for the 2Co/2Pt system with Stoner enhancement in Pt turned on (black line) and off (red line) as a function of energy $E = \hbar\Omega$.

effect on the damping rate in the Co/Pd(001) system. In the presence of SOC, however, the effect can be very large indeed. Both magnetocrystalline anisotropy and damping rate are significantly different in the enhanced and nonenhanced cases, as shown in Fig. 6. The Gilbert parameter is also very different in the two cases: $\alpha_G^{\mathrm{enh}} = 0.11$, whereas $\alpha_G^{\mathrm{non-enh}} = 0.33$. Thus, proper treatment of Stoner enhancement in substrates like Pd and Pt is essential for the correct determination of spin relaxation features.

We presented a microscopic scheme for calculating the Gilbert damping parameter α_G in ultrathin metallic magnetic films, and illustrate it by presenting results for unsupported Co films and for Co/Pt bilayers. Our approach is based on the evaluation of the dynamic transverse susceptibility in the presence of spin-orbit coupling, taking into account realistic electronic structures and the coupling between transverse spin, longitudinal spin, and charge excitations. The essential difference between our approach and the ones usually found in the literature is the description of the magnetization dynamics in terms of collective spin excitations. As a consequence we find finite values of α_G in the limit of perfectly crystalline films, a regime where methods based on the torque correlation formula find a diverging Gilbert damping parameter. We showed that the coupling between transverse, longitudinal, and charge excitations, due to spin-orbit coupling, is of fundamental importance for the correct determination of FMR spectra in metallic systems. We have also shown that the damping rate extracted from the FMR spectrum for a fixed excitation frequency may differ considerably from that extracted from the FMR spectrum for a fixed Zeeman field. In this case the Gilbert damping parameter α_G becomes frequency dependent, in contrast to what is assumed in the standard Landau-Lifshitz-Gilbert phenomenology. Moreover, we have numerical indications that the Gilbert parameter may not be well defined in the limit of vanishing resonance frequency, a fact that is very relevant to calculational schemes based on the adiabatic approximation. Incidentally, Stoner enhancement in materials like Pt and Pd also plays an important role in the determination of FMR frequencies and damping rates. These results may lead to important modifications of the interpretation of damping parameters, either calculated or inferred from experimental results, for systems where spin-orbit coupling is strong. We believe these issues may be crucial for the correct description of relaxation in very clean systems of nanoscopic dimensions, especially in the presence of relatively weak magnetocrystalline anisotropy.

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