Spin-orbital Gilbert damping in common magnetic metals

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Understanding the damping of fast magnetization precession in ferromagnetic metals is important for many applications. Spin-orbital effective fields fluctuating as a result of electron collisions with the lattice defects are known to cause magnetic damping of the Gilbert type. Formulas convenient for numerical estimates derived using exact linear-response theory are discussed in terms of the Fermi golden rule. Estimates of the damping rates in Fe and Ni based on band structures matched to *ab initio* calculations and on the lifetime approximation account for a substantial part of the experimental values. The relevance of the lifetime approximation is discussed and supported by a simple model calculation.

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I. INTRODUCTION

General interest in the damping of fast magnetization precession has been revived by projects of fast memories employing films of magnetic metals. While immediate interest seems to concentrate on nonlocal damping effects in ultrathin film structures,[1,2] such experiments also detect the local "intrinsic" Gilbert damping, known in bulk ferromagnetic resonance[3–9] (FMR) and usually described by the last term in the equation of motion[10] for the magnetization **M**,

$$\frac{d\mathbf{M}}{dt} = -\gamma[\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}] + \alpha\left[\frac{\mathbf{M}}{M_s}\times\frac{d\mathbf{M}}{dt}\right]. \qquad (1)$$

Here, $\mathbf{H}_{\mathrm{eff}}$ is the "effective" magnetic field (including the Maxwell **H** and effects of macroscopic magnetic anisotropy), $\gamma>0$ is the gyromagnetic ratio, M_s is the saturation magnetization, and α is the damping parameter, often measured in terms of the Landau-Lifshitz damping rate[6] $\lambda=\alpha\gamma M_s$ (in cgs units).

Since uniform precession is not affected by isotropic exchange interaction, the source of the Gilbert damping has been sought in magnetic forces. Dipolar damping is generally associated with nonuniform magnetization and at least qualitatively understood in terms of scattering into nonuniform magnons.[11] The role of spin-orbit coupling (SOC) in magnetic 3*d* metals had been schematically described by Brooks.[12] Orbital moments quenched by electron itinerancy[13] are only partly, weakly restored by SOC and depend on the prevalent spin direction as well as on the direction of the electron wave vector **k**. Thus, orbital moments of itinerant electrons change as **M** turns and also when **k** is changed in collisions with lattice defects. Random scattering is, thus, a source of noise in the effective SOC fields acting on the spin system, similarly as in electron spin resonance of conduction electrons in simple metals.[14–16]

Unfortunately, we can, so far, only roughly estimate the range of itinerant lifetimes (from the resistivity), but not yet include a specific scattering mechanism in a realistic detailed theory.

It was, nevertheless, possible to estimate the influence of electron lifetimes at the Fermi level on the Gilbert damping caused by oscillating electron levels[17–20] as well as by oscillating orbital polarization[20–22] (i.e., oscillation of the mean-field Hamiltonian, not only of the energy values). The common features of these estimates had been, on the one hand, more or less accurate calculations of the frequency spectra of the effective SOC fields, including interband excitations at low optical frequencies, in the band structures of ideal crystals and, on the other hand, phenomenologically expected change of these spectra when the energy levels are broadened due to finite lifetimes of the electron states.

While the inaccuracy of earlier quantitative estimates has been recently removed,[18–20] there remain several points where an improved presentation may foster better general understanding of the subject and provoke further theoretical progress.

In the presented work, we try (i) to simplify the derivation of the torque correlation formula[21] used in the numerical estimates, particularly the inclusion of interband excitations; (ii) in this context and in connection with different formulations[2,23,24] and with numerical calculations, to distinguish the roles of several types of interband excitations (that may mainly change the spin or orbital state, or both); and, finally, (iii) to discuss the relevance and limitations of the lifetime approximation (LTA) in relation to various types of interband polarizations. The last point caused an early controversy[24–26] and was most neglected in all previous treatments of the subject. It may also be important for explaining the remaining differences between theoretical and experimental results.

Since our main objective is to contribute to general, at least qualitative, understanding, we use elementary argument where possible, particularly the Fermi golden rule in Sec. II and in the rather extended discussion in Sec. IV. In Sec. III, we revise our previous numerical results[17,21,22] by improved calculations (employing *ab initio* energy spectra). We refer to established linear-response and Green's function methods in Appendix A for support of the golden-rule approach of Sec. II, and in Appendix B for the LTA of Sec. III and of the necessary (vertex) corrections, which are only briefly discussed in Sec. IV B. These technical matters are formulated differently by other authors. We also try to show, on a simple point-defect model, that the (vertex) correction to LTA does not diminish the damping derived from interband SOC excitations, although it is known to invalidate the simple LTA in models with effective fields derived from isotropic exchange.

II. ELEMENTARY FORMULATION

Interaction of the collective magnon mode with electrons near the Fermi level may be phenomenologically described by an effective Hamiltonian[17,27]

$$H_{me} = \omega b^\dagger b + \sum_{\mu\nu} (E_\mu \delta_{\mu\nu} + \phi^\dagger_{\mu\nu} b + \phi_{\mu\nu} b^\dagger) c^\dagger_\mu c_\nu, \tag{2}$$

where b^+ (b) and c^+_μ (c_μ) create (annihilate) uniform magnons and electrons in states $|\mu\rangle$. All energy variables like H, E, and ϕ will be assumed in units of frequency (divided by $\hbar$). The interaction elements may be derived from the equations of motion (used in linear-response theory, cf. Appendix A). The uniform magnon is a quantum of electron spin deviation,

$$b_e = N_s^{-1/2} \sum_{\mu\nu} S^-_{\mu\nu} c^\dagger_\mu c_\nu, \tag{3}$$

where S^- is in units of $\hbar$ and $N_s = -2\langle \Sigma_{\mu\nu} S^z_{\mu\nu} c^+_\mu c_\nu \rangle_{e,c}$. The symbol $\langle\ \rangle_{e,c}$ denotes macroscopic average over electron and lattice states.[28] We require that the right-hand side of $i\partial b/\partial t = [b, H_{\rm me}]$ from Eq. (2) be equal to $[b_e, H_{\rm el}]$, where $H_{\rm el}$ is the full (many-body) electron Hamiltonian. The only two terms in $H_{\rm el}$ that do not commute with the total spin are the SOC, $H_{\rm so}$, and the dipolar interactions. Ignoring the latter [or including them in macroscopic $H_{\rm eff}$ in Eq. (1)], we get

$$\phi_{\mu\nu} = N_s^{-1/2} F^-_{\mu\nu}, \tag{4a}$$

$$F^-_{\mu\nu} = [S^-, H_{\rm so}]_{\mu\nu}. \tag{4b}$$

SOC is well represented by the one-electron operator

$$H_{\rm so} = \xi \mathbf{L} \cdot \mathbf{S}, \tag{5a}$$

$$\xi \mathbf{L} = \sum_j \xi_j \mathbf{L}_j, \tag{5b}$$

where $\mathbf{L}_j$ denotes electron orbital angular momentum with respect to atom site j, and ξ_j is a scalar functional[29,30] or its average value in simplified models.[12,31] Following Eqs. (4) and (5),

$$F^-_{\mu\nu} = (\xi L_z S^- - \xi L^- S_z)_{\mu\nu}. \tag{6}$$

The Fermi golden rule determines the magnon creation and destruction rates, p^+ and p^-, as

$$p^\pm = 2\pi \Big\langle \sum_{\mu\nu} |\langle n_b \pm 1; n_\mu + 1, n_\nu - 1 | H_{\rm me} | n_b; n_\mu, n_\nu \rangle|^2 \times \delta(E_\mu - E_\nu \pm \omega) \Big\rangle_{e,c}, \tag{7}$$

where n_b and n_μ are the magnon and electron occupation numbers. The average $\langle\ \rangle_{e,c}$ will be taken separately over the electron (e) degrees of freedom and then over the lattice configurations (c) affected by disorder. The δ function and the subsequent treatment correspond to the basic adiabatic approximation.

The squared element of $c^+_\mu c_\nu$ alone is $(1-n_\mu)n_\nu$, while b^+ (b) give $1+n_b$ (n_b) in p^+ (p^-). Swapping μ and ν in p^+, we get the net p^- and p^+ with the same $|\phi^+_{\mu\nu}|^2$ and δ factors. Assuming that electrons remain in equilibrium, i.e., the mean $\langle n_\mu \rangle_e$ equal $f_\mu = f(E_\mu)$, where $f(E) = \{1 + \exp[(E-E_F)/kT]\}^{-1}$ is the Fermi function, and using the identity $(1-f_\nu)f_\mu = (f_\nu - f_\mu)g(E_\mu - E_\nu)$, where $g(E)$ is the Bose function $\{1 - \exp(E/kT)\}^{-1}$, we get the net rate

$$p^- - p^+ = \frac{n_b - n_{b0}}{\tau_b},$$

$$\frac{1}{2\pi\tau_b} = \Big\langle \sum_{\mu\nu} |\phi^\dagger_{\mu\nu}|^2 (f_\nu - f_\mu)\, \delta(E_\mu - E_\nu - \omega) \Big\rangle_c \tag{8}$$

where $n_{b0} = g(\omega)$ is the equilibrium magnon number and $1/\tau_b$ is the magnon decay frequency.[27]

Since the Gilbert equation (1) gives $\alpha\omega$ for the decay rate of linear magnetization deviations $\delta\mathbf{M}$, while $1/\tau_b$ describes the decay of magnon numbers, i.e., of $(\delta\mathbf{M})^2$, the Gilbert α may be identified with $1/2\omega\tau_b$ or, strictly, with the limit $\partial(1/2\tau_b)/\partial\omega$ at $\omega = 0$. This limit is

$$\alpha = \pi \Big\langle \sum_{\mu\nu} |\phi^\dagger_{\mu\nu}|^2 \eta(E_\nu)\, \delta(E_\mu - E_\nu) \Big\rangle_c, \tag{9}$$

with $\eta(E) = -\partial f(E)/\partial E$ peaked at the Fermi level E_F.

For a discussion of lattice disorder, it is useful to separate the explicit dependence on the temperature in the Fermi factor $\eta(E)$ and the normalizer N_s (proportional to M_s), writing Eq. (9) as $\alpha = \int \eta(E) \alpha_E dE$,

$$\alpha_E = \pi \Big\langle \sum_{\mu\nu} |\phi^\dagger_{\mu\nu}|^2 \delta(E - E_\mu)\, \delta(E - E_\nu) \Big\rangle_c \tag{10a}$$

$$= \pi N_s^{-1} \langle \mathrm{Tr}\{F^+ D(E) F^- D(E)\} \rangle_c, \tag{10b}$$

where $D(E)$ is the spectral density matrix:

$$D(E)_{m\mathbf{k},n\mathbf{k}'} = \sum_\mu U_{m\mathbf{k},\mu} \delta(E - E_\mu) U^\dagger_{\mu,n\mathbf{k}'}, \tag{11a}$$

$$|\mu\rangle = \sum_{m\mathbf{k}} |m\mathbf{k}\rangle U_{m\mathbf{k},\mu}, \tag{11b}$$

if the states $|\mu\rangle$ needed for the exact energy balance are regarded as (so far unknown) mixtures of the Bloch states $|m\mathbf{k}\rangle$ of an ideal crystal.

III. LIFETIME APPROXIMATION

Band calculations in pure metals give us only the periodic part of $F^\pm$, diagonal in the wave vector $\mathbf{k}$, and allow us to estimate only the *averaged* spectral densities of individual band states as

$$\langle D(E)_{m\mathbf{k}} \rangle_c = \frac{1}{\pi} \frac{w_{m\mathbf{k}}}{(E - E_{m\mathbf{k}})^2 + w^2_{m\mathbf{k}}}. \tag{12}$$

A single index is used for diagonal elements, and the Bloch level width $w_{m\mathbf{k}} = (2\tau_{m\mathbf{k}})^{-1}$ is related to the Bloch state lifetime, $\tau_{m\mathbf{k}}$. Using only these averages instead of the D matrices in Eq. (10) yields the lifetime approximation

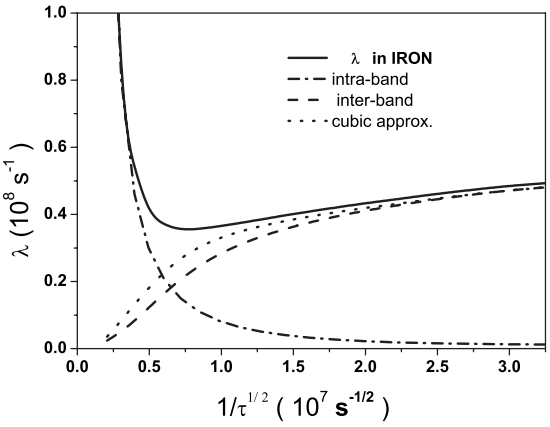

FIG. 1. Calculated Landau-Lifshitz damping rate λ for iron (solid line) as function of the electron lifetime τ (note the nonlinear $\tau^{-1/2}$ scale). The intraband (dashed-dot line) and interband (dashed line) components of λ and the cubic approximation (dotted line) are discussed in the text.

$$\alpha_E^{(L)} = \pi N_s^{-1} \sum_{m\mathbf{k},n} |F^+_{m\mathbf{k},n\mathbf{k}}|^2 \langle D(E)_{m\mathbf{k}} \rangle_c \langle D(E)_{n\mathbf{k}} \rangle_c, \qquad (13)$$

which may be evaluated numerically as a function of the lifetimes $\tau_{m\mathbf{k}}$ regarded as free parameters.

The damping parameters calculated for iron and nickel are shown in Figs. 1 and 2. The energy spectrum $E_{m\mathbf{k}}$ was calculated using the *ab initio* WIEN2K package,[30] and the summation (13) was done using interpolation schemes [of ten 3*d* linear combination of atomic orbitals (LCAO) bands hybridized with eight orthogonal plane wave bands, as designed by Hodges *et al.*[32] for fcc Ni and adapted[33] for bcc Fe]. SOC was included as defined in Eqs. (5) and (6), with **L** elements[31] taken only between the 3*d* LCAO and the SOC parameters ξ matched to the $X_{25'}$ splitting in Ni and $H_{25'}$

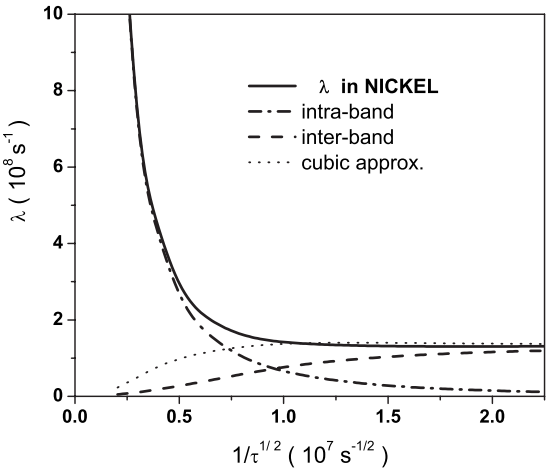

FIG. 2. Calculated Landau-Lifshitz damping rate λ for nickel (solid line) as function of the electron lifetime τ (note the vertical scale 10× larger than in Fig. 1). The intraband (dash-dot line) and interband (dashed line) components of λ and the cubic approximation (dotted line) are discussed in text.

splitting in Fe in the WIEN2K spectra. Except for the variable τ, substituted as a single free parameter for all unknown $\tau_{m\mathbf{k}}$, there remained no adjustable parameters.

The vertical axes in Figs. 1 and 2 show the frequency $\lambda = \alpha\gamma M_s$ (in cgs units), which is more common in experimental literature and more conveniently normalized (the Gilbert α contains the temperature-dependent M_s due to $N_s^{-1} = \gamma\hbar/2M_s\Omega$, with Ω for the normalization volume). The formula used in the calculation takes for α only $\alpha_E^{(L)}$ from Eq. (13) at the Fermi level E_F, i.e.,

$$\lambda = \frac{\gamma^2\hbar}{2\pi\Omega_{at}} \left\langle \sum_{m,n} |F^+_{m\mathbf{k},n\mathbf{k}}|^2 \frac{w}{E'^2_{m\mathbf{k}} + w^2} \frac{w}{E'^2_{n\mathbf{k}} + w^2} \right\rangle_{\mathbf{k}}. \qquad (14)$$

Here, Ω_{at} is the atomic volume, $\langle\ \rangle_{\mathbf{k}}$ denotes an average over the first Brillouin zone, $E' = E - E_F$, and $w = (2\tau)^{-1}$ is a free parameter replacing the unknown $w_{m\mathbf{k}}$ in Eq. (12).

The horizontal axis in Figs. 1 and 2 is linear in $\tau^{-1/2}$ in order to facilitate comparison with the experimental plots[5–9] of λ against the temperature, T; it may be assumed that $1/\tau$ is proportional to the resistivity, which, in turn, is proportional[7] to T^2.

Besides the total λ, the figures also show separately the contributions of intraband terms (diagonal, $m=n$, dashed-dot lines), apparently dominant at low $1/\tau$, and the interband contributions [off-diagonal, $m \neq n$ in Eqs. (13) and (14), dashed lines] that initially increases with $1/\tau$, but then, more or less, saturate, particularly in Ni.

The dotted lines in Figs. 1 and 2 are plots of λ in the cubic approximation, which includes SOC in $F_{m\mathbf{k},n\mathbf{k}}$ elements but not in the $E_{m\mathbf{k}}$ spectra, and appears to be sufficient for high $1/\tau$. This approximation allows us to distinguish spin-down and spin-up bands, and to separate the contributions of the $\xi L_z S^+$ and $\xi L^+ S_z$ excitations constituting $F^{\pm}$ [cf. Eq. (6)]. In Ni, the largest share in the calculated λ comes from the essentially *orbital* excitations $\xi L^+ S_z$ in the prevalent minority-spin (up) states at the Fermi level. In Fe, a great part (about 2/3) of λ at high $1/\tau$ is due to *spin* excitations $\xi L_z S^+$ (between orbitally different states, not to be confused with *pure* spin Stoner excitations).

IV. DISCUSSION

A. Effective field elements

The magnon-electron interaction in Eq. (2) may be interpreted as a variation of the mean-field Hamiltonian H_{mf} of electrons (near the Fermi level) caused by a small angular deviation $\delta\mathbf{m}$ of the magnetization direction $\mathbf{m} = \mathbf{M}/M_s$ from the static position $\mathbf{m}_o = \mathbf{z}$. The last term in Eq. (2) may be written as

$$\delta H_{\mathrm{mf}} = -\mathbf{F} \cdot \delta\mathbf{m}, \qquad (15)$$

where $\delta\mathbf{m}$ is regarded as a dynamic variable represented by magnon operators,[11] $\delta m^x - i\delta m^y \to -2N_s^{-1/2} b$, and $\mathbf{F}$ has only components transverse to $\mathbf{z}$: following Eq. (6), for $F^- = F_x - iF_y$,

$$\mathbf{F} = [\xi \mathbf{L} \times \mathbf{S}] \times \mathbf{m}_o. \tag{16}$$

On the other hand, the effective magnetic field acting on the collective magnetization is represented by the electron operator $\mathbf{h}_{\rm ef}$ determined from

$$\gamma \mathbf{h}_{\rm ef} = \frac{2}{N_s} \sum_{\mu\nu} \mathbf{F}_{\mu\nu} c_\mu^\dagger c_\nu \tag{17}$$

(if again $H_{\rm mf}$ and $\mathbf{F}$ are in frequency units and $N_s = 2M_s\Omega/\hbar\gamma$). The connection of the Gilbert damping with the formal theory of effective field fluctuation was recently reviewed by Heinrich.[2] In the present approximation, we get from Eq. (8) for $\alpha = 1/2\omega\tau_b$ at finite ω

$$\begin{aligned}\alpha(\omega) &= \frac{\pi}{\omega} \left\langle \sum_{\mu\nu} |\phi_{\mu\nu}^+|^2 (f_\nu - f_\mu) \delta(E_\mu - E_\nu) \right\rangle_c \\ &= \frac{1}{2\omega N_s} \int_{-\infty}^{\infty} \langle [F^-(t), F^+] \rangle_{e,c} e^{i\omega t} dt \\ &= \frac{1}{2N_s} \int_{-\infty}^{\infty} \int_0^\beta \langle F^-(t - is) F^+ \rangle_{e,c} ds e^{i\omega t} dt, \end{aligned} \tag{18}$$

where $(F(t))_{\mu\nu} = F_{\mu\nu} \exp[i(E_\mu - E_\mu)t]$ in the second line, giving the spectral density of the retarded function[34,35] derived in Appendix A. The form of the third line where $\beta = \hbar/k_B T$ is obtained as one of the well-known Kubo identities[34,36] for averages over canonical distributions. It also follows from the formal fluctuation theory,[36] where, however, the $F(t)$ dependence contains only random field, from which all projections onto the collective magnon mode are removed.[36] In the present simplified formulation giving the second and first lines, the damping results from energy and angular momentum transfer to electron-hole excitations, with the dynamics described by the *static* $H_{\rm mf}$ in which low-frequency magnons do not exist.

The variational form of $\delta H_{\rm mf}$ has been derived earlier in two different ways. It has been noted that Eq. (15) with Eq. (16) is the variation of the SOC Hamiltonian,[17,29] i.e., $\delta H_{\rm mf} = \delta H_{\rm so}$, because the form of $H_{\rm so}$ varies[31] when spin variables are written in the *rotating frame*, with the spin quantization axis (time-dependent z' axis) following the magnetization direction $\mathbf{m}$ but orbital variables in the static frame.

On the other hand, in earlier formulations,[24,37] variation of the electron mean field caused by $\delta\mathbf{m}$ is naturally derived from the *rotating mean exchange field* acting on the electrons in the *static frame*. If the mean exchange field is schematically described by $H_{\rm ex} = \Delta \mathbf{S} \cdot \mathbf{m}$, where $\Delta = \Sigma \Delta_a |a\rangle\langle a|$ is a Stoner splitting operator,[38] the static part $H_{\rm ex}^0 = \Delta S_z$ is included in $H_{\rm mf}$, while the dynamic part is

$$\delta H_{\rm ex} = \Delta \mathbf{S} \cdot \delta \mathbf{m}. \tag{19}$$

Quantized $\delta\mathbf{m}$ renders the interaction term in Eq. (2) with matrix elements, instead of Eqs. (4) and (6),

$$\phi_{\mu\nu}^{(ex)} = -N_s^{-1/2} (\Delta S^-)_{\mu\nu}. \tag{20}$$

These elements joining states of opposite spin across the Stoner gaps are clearly different from Eqs. (4) and (6). Thus, it is necessary to recall that the equations of motion used in Sec. II and the energy conservation condition strongly restrict the choice of exchange-field elements that contribute to the damping. Isotropy of exchange implies that $(\Delta S^-)_{\mu\nu}$ is equal to $[S^-, H_{ex}^0]_{\mu\nu}$, while

$$[S^-, H_{ex}^0 + H_{so} + H_z]_{\mu\nu} = (E_\nu - E_\mu) S_{\mu\nu}^-$$

for elements between the static eigenstates. In particular, for the states involved in the "golden rule" Eq. (7), the right-hand side is equal to $\omega S_{\mu\nu}^-$ and to the Zeemann term $[S^-, H_z]_{\mu\nu}$. Hence, $(\Delta S^-)_{\mu\nu} = -F_{\mu\nu}^-$ and the $\phi_{\mu\nu}$ elements from Eq. (20) and from Eq. (6) are the same. This is particularly true for the diagonal (intraband) elements contributing to the damping in the theory of Korenman and Prange[24,26] and in the "breathing Fermi surface" model.[18,19]

The role of interband matrix elements in the lifetime approximation is discussed in more detail further below. Both $H_{\rm so}$ and $F^\pm$ are strictly off-diagonal in the Bloch states[31,32]

$$|as\mathbf{k}\rangle = \sum_\alpha C_{as\mathbf{k}}^\alpha N_{at}^{-1/2} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} |\alpha j\rangle |s\rangle, \tag{21}$$

with fixed spin labels s, containing atomic orbitals $|\alpha j\rangle$, where j denotes the $\mathbf{r}_j$ site and α one of the *real* $3d$ wave functions. The Cartesian L^r components $(r = x, y, z)$ are off-diagonal in such atomic orbital (AO) basis as well as in the LCAO as long as $C_{as\mathbf{k}}^\alpha$ are also real (i.e., before including $H_{\rm so}$ in $H_{\rm mf}$). Thus, $F^\pm$ connect LCAO states with different orbital parts so that the space of SOC field excitations (17) is separated from the spin-wave operator space.

This concerns also the $L_z S^\pm$ part of the field elements, between bands of opposite spin but also of different orbital (AO) compositions. According to the numerical estimates in Sec. III, these "spin-spin" excitations cause approximately 2/3 of the damping in Fe at high τ^{-1}, where λ is simply proportional to ξ^2. This proportionality is pointed out by Heinrich[2] in a formula[39] for λ that is recently used and discussed in context with experiments supporting such proportionality.[23] The quoted formula[2,39] is, however, based on a truncated magnon-electron interaction, with F^- in $H_{m\text{-}e}$ reduced to the $S_z L^-$ terms. This resulted from regarding only the transverse $r = x$ and y in $H_{\rm so} = \Sigma \xi L_r S_r$ as in electron paramagnetic resonance (EPR) damping,[14–16] also quoted in the *sd* model.[37] There is, however, no obvious reason for neglecting the "secular" term $(r = z)$ in $H_{\rm so}$, leading to a spin-spin process of scattering collective magnon to electron-hole pairs of opposite spins combined with orbital L_z excitation. It is similar to the two-magnon process caused by random local h_z fields.[11,40] While fluctuations of the transverse $L_r S_r$ components are known to cause EPR and also NMR damping,[41] the secular spin-orbital terms $\xi L_z S_z$ must, intuitively, cause slight dephasing of spin excitation of Bloch states during their short lifetime.

The present discussion is deliberately limited to *local* damping of uniform precession. The damping of nonuniform spin waves represented by spatially modulated operators $S_{\mathbf{q}}^- = S^- e^{i\mathbf{q}\cdot\mathbf{r}}$ has two additional features. The spin-orbital effective-field operators (4b) are also spatially modulated; they have no strictly diagonal elements in the Bloch representation, and the breathing Fermi surface mechanism analo-

gous to the Drude-Sommerfeld picture of electromagnetic wave absorption is modified to direct absorption analogous to Pippard's "anomalous" skin effect[17,24] if the electron mean free path is longer than the spin wave length. Second, the nonuniform $S_{\mathbf{q}}^{-}$ does not commute with electron *kinetic* energy so that the effective field contains, besides the magnetic F^{-} from Eq. (4b), also diffusive terms $\mathbf{q}\cdot\mathbf{v}S_{\mathbf{q}}^{-}$, where $\mathbf{v}$ is the electron velocity. The matrix elements of this diffusive "force" join states with opposite spins and (nearly) the same orbital parts, like the Stoner S^{-} excitations. The resulting diffusive damping is small in usual skin-effect conditions in ferromagnetic resonance, but its importance increases in heterostructures with ultrathin ferromagnetic components.[2] This *nonlocal* damping is, of course, not described by the macroscopic Gilbert equation.

B. Lifetime approximation and corrections

As in EPR damping,[14–16] we should consider two sources of randomness and noise in effective-field excitations. One is disorder in SOC, which might be represented by a local variation of ξ_i parameters. The other is ordinary scattering, which also causes electrical resistance. An obvious weakness of the present LTA is in neglecting the local variation of H_{so} and $\mathbf{F}$, regarded as periodic operators (diagonal in $\mathbf{k}$). The calculated damping is, thus, certainly underestimated.

Another less obvious weakness with possibly serious consequences is the severe truncation of interfering scattering amplitudes between different bands, implied by using in Eq. (13) only the average diagonal elements of the spectral densities (12), instead of all the interfering elements (11a) contained in Eq. (10b).

The finite lifetimes of the Bloch states result from scattering by aperiodic perturbation potential, say, V, superposed on the average periodic mean field. Relations between the scattering amplitudes, the spectral density matrix, and the averages needed in Eq. (10b) are usually treated by perturbation theory for complex transforms of $D(E)$ (as recalled in Appendix B). The essence of the implicit truncation in the LTA is clearly seen in the simple first Born approximation, substituting for $|\mu\rangle$ in Eq. (11b) only weakly perturbed Bloch states,

$$|\tilde{m}\mathbf{k}\rangle = |m\mathbf{k}\rangle + \sum_{p\mathbf{k}'} |p\mathbf{k}'\rangle \frac{V_{p\mathbf{k}',m\mathbf{k}}}{E_{m\mathbf{k}} - E_{p\mathbf{k}'}}. \tag{22}$$

The F^{+} elements between such states are, for $\mathbf{k}' \neq \mathbf{k}$ and to first order in V,

$$F^{+}_{\tilde{p}\mathbf{k}',\tilde{n}\mathbf{k}} = \sum_{m} \frac{V_{p\mathbf{k}',m\mathbf{k}} F^{+}_{m\mathbf{k},n\mathbf{k}}}{E_{m\mathbf{k}} - E_{p\mathbf{k}'}} + \sum_{q} \frac{F^{+}_{p\mathbf{k}',q\mathbf{k}'} V_{q\mathbf{k}',n\mathbf{k}}}{E_{n\mathbf{k}} - E_{q\mathbf{k}'}}. \tag{23}$$

Substituting their absolute squares to Eq. (10a), we get the LTA for α if, among all the various products of V elements, we keep *only* the absolute squares $|V_{p\mathbf{k}',m\mathbf{k}}|^2$, i.e., only the absolute squares of the individual terms in Eq. (23) in the averages $\langle\ \rangle_c$. We also neglect perturbation of the energy values, note that $|F^{+}_{p\mathbf{k}',q\mathbf{k}'}|^2$ equals $|F^{-}_{q\mathbf{k}',p\mathbf{k}'}|^2$, and express both in terms of the Hermitian rectangular components F^r, $r=x$ and y in Eq. (16). We note [cf. also Eq. (B7) in Appendix B] that

$$2\pi \left\langle \sum_{p\mathbf{k}'} |V_{p\mathbf{k}',m\mathbf{k}}|^2 \delta(E - E_{p\mathbf{k}'}) \right\rangle_c = \frac{1}{\tau_{m\mathbf{k}}} \tag{24}$$

is the golden-rule probability of scattering from $|m\mathbf{k}\rangle$ to the states at level E, and get

$$\alpha_E^{(L)} = N_s^{-1} \sum_{n\mathbf{k},m,r} \frac{|F^r_{n\mathbf{k},m\mathbf{k}}|^2 \delta(E_F - E_{n\mathbf{k}})}{(E_{m\mathbf{k}} - E_{n\mathbf{k}})^2 \tau_{m\mathbf{k}}}. \tag{25}$$

The same result for α is obtained from Eq. (13), with the averaged spectral densities following Eqs. (11a), (11b), and (22), with $\langle V\rangle_c = 0$,

$$\langle D(E)_{m\mathbf{k}}\rangle_c = \delta(E - E_{m\mathbf{k}}) + \frac{(2\pi\tau_{m\mathbf{k}})^{-1}}{(E - E_{m\mathbf{k}})^2}. \tag{26}$$

This approximate $\langle D\rangle_c$ is singular at $E=E_{m\mathbf{k}}$ and obviously not normalized (the integral over E is not unity), as a result of failure to subtract the density scattered *from* the peak at $E=E_{m\mathbf{k}}$ into the "tail," and failure to take into account also energy variations. These failures are corrected in the improved approximation recalled in Appendix B, leading to Lorentzian $\langle D\rangle_c$ used in Eq. (12). Without this correction, Eqs. (22)–(26) are only applicable and may be used for the discussion of *interband* $F^{\pm}$ contributions.

Summation of *all* averages $\langle V_{m\mathbf{k},p\mathbf{k}'} V_{q\mathbf{k}',n\mathbf{k}}\rangle_c$ contained in the mean absolute square of the elements (23) would be equivalent to including *off-diagonal* elements of the D matrices in Eq. (10b), at least to first order in V:

$$D^{(1)}_{m\mathbf{k},n\mathbf{k}'} = V_{m\mathbf{k},n\mathbf{k}'} \left[\frac{\delta(E - E_{m\mathbf{k}})}{E - E_{n\mathbf{k}'}} + \frac{\delta(E - E_{n\mathbf{k}'})}{E - E_{m\mathbf{k}}} \right] \tag{27}$$

[cf. also Eq. (B6a), second term]. Such complete summation requires more effort and also knowledge of V.

The following tractable example shows the importance of checking the LTA in the *s-d* models and other formulations using effective-field elements derived from isotropic exchange interactions. With $\phi^{(ex)}$ elements from Eq. (20), the LTA predicts spurious damping from overlapping densities of $\uparrow$ and $\downarrow$ spin states, i.e., α from Eq. (25) with F^r replaced by ΔS^r and $E_{m\mathbf{k}} - E_{n\mathbf{k}}$ equal to the exchange gap. This damping would persist even without SOC. However, it may be readily shown that the averages $\langle D^{(1)}\phi^{ex}D^{(1)}\rangle_c$ with spin-independent V elements in Eq. (27) cancel the $\langle D\rangle_c$ overlap terms from Eq. (13), so that the result in Eq. (10b) is 0. In simpler terms, the relevant $\phi^{(ex)+}$ elements (23) between the Born states (22) with sharp orbital labels a and b and spin labels $s=\downarrow$ and $\uparrow$ vanish:

$$\langle \tilde{b}\uparrow\mathbf{k}'|\Delta S^{+}|\tilde{a}\downarrow\mathbf{k}\rangle = \frac{V_{b\uparrow\mathbf{k}',a\uparrow\mathbf{k}}\Delta_{a\mathbf{k}}}{E_{b\uparrow\mathbf{k}'} - E_{a\uparrow\mathbf{k}}} + \frac{\Delta_{b\mathbf{k}'} V_{b\downarrow\mathbf{k}',a\downarrow\mathbf{k}}}{E_{a\downarrow\mathbf{k}} - E_{b\downarrow\mathbf{k}'}}$$

equals 0 due to isotropy of exchange, for the low-energy transitions where $E_{a\downarrow\mathbf{k}} = E_F = E_{b\uparrow\mathbf{k}'}$, the two energy denominators equal $-\Delta_{a\mathbf{k}}$ and $\Delta_{b\mathbf{k}'}$, respectively, and the V elements are the same.

Korenman and Prange[24,26] refer to exchange-field elements in LTA, but avoided the "spurious overlap" error by

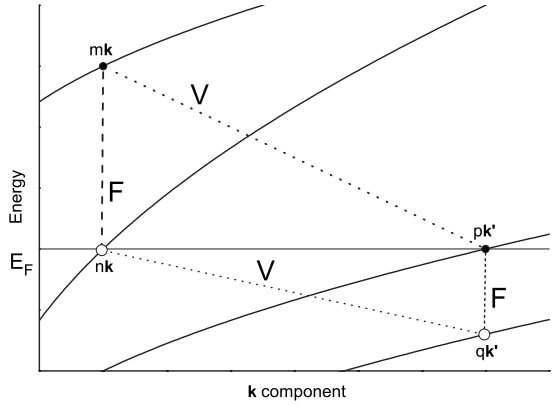

FIG. 3. Schematic illustration of electron-hole pair ($n\mathbf{k}-p\mathbf{k}'$) generated by combined interband polarization F and scattering by defect V. The lifetime approximation neglects correlation between $V_{m\mathbf{k},p\mathbf{k}'}$ and $V_{n\mathbf{k},q\mathbf{k}'}$ elements.

reducing "relevant" elements to those diagonal in the band number index (equal to the SOC elements).

Most versions[37,42] of the *s-d* model avoid such overlap error by using a different LTA, referring explicitly to *spin lifetime* ascribed to SOC of the *s-p* states[2,37] or to impurities,[42] but the present form of Eq. (13) with Eq. (12) and isotropic exchange, instead of SOC elements for F assumed in another recent version,[43] is not so realistic.

Figure 3 schematically illustrates the generation of an electron-hole pair at E_F caused by the electron-magnon interaction F combined with scattering by random V.

In the preceding example, m and p denote $\uparrow$ spin bands and n,q denote $\downarrow$ spin bands; a $F^{(ex)}_{m\mathbf{k},n\mathbf{k}}$ excitation at $\mathbf{k}$ may be destroyed by $V_{p\mathbf{k}',m\mathbf{k}}$, but this is not sufficient to cause magnetic damping, because the interfering $V_{n\mathbf{k},q\mathbf{k}'}$ restores a $F^{(ex)}_{p\mathbf{k}',q\mathbf{k}'}$ excitation at $\mathbf{k}'$, so that total spin is (naturally) conserved. In this case, there is strong correlation between the $F^{(ex)}$ elements and the energy gaps, and also between the two V elements.

Analogous interference should not be *a priori* ignored in the case of spin-orbital fields F, but the result is quite different. It is again best visible in the structure of approximate $|as\mathbf{k}\rangle$ bands (21) without SOC (with no *intraband F* elements and the interband F connecting different orbital states). Variation of the $F_{bs'\mathbf{k},as\mathbf{k}}$ elements, with $\mathbf{k}$ running over the 48 values in the cubic star of $\mathbf{k}$, is determined by variation of the $L^r_{b\mathbf{k},a\mathbf{k}}$ elements, and that, in turn, is the variation of axial vector components (in particular, the $L^r_{b\mathbf{k},a\mathbf{k}}$ elements of all three components, $r=x,y,z$, attain the same set of values in the star). This variation is completely decoupled from the behavior of the interband energy gaps since $E_{as\mathbf{k}}$ are invariant in the star. This feature led to the assumption[21,26] that the F elements are, generally, not conserved in V scattering and that the correction to LTA is negligible.

To support or falsify this assumption, the correction had been estimated[22] in a simple model of point-defect scattering, which conserves L^r at each scattering site, but L^r elements between the Bloch states are dispersed due to their dependence on the direction of propagation, $\mathbf{k}$. This model is hardly appropriate for thermal (phonon) deformation, but it is the simplest available for a qualitative discussion of "vertex" corrections. In addition, it may simulate scattering effects in alloys, such as 5% Cu in Ni in the remarkable experiment that had most strongly supported the role of itinerant electron scattering in the Gilbert damping.[6,24,44]

The calculation is particularly simple for the truncated $3d$ model, consisting only of the six bands composed of the three t_{2g} orbitals (considered by Brooks[12] for magnetic anisotropy and by Obata[41] for NMR relaxation by orbital L^r fluctuations). The calculation is presented in Appendix B in the Green's function formalism that parallels the present Born approximation. This approximation led earlier[22] to a simple result for α due to same-spin (s) elements $\xi S_z L^{x,y}$ [that have the same mean squares in the star, for any pair of band indices $a \neq b$; cf. also Eqs. (B13) and (B17)]:

$$\alpha_{E,s} = \tau_s^{-1} N_s^{-1} Z_s(E)(\xi^2/3)(\langle \epsilon_s^{-2} \rangle + \langle \epsilon_s^{-1} \rangle^2), \tag{28}$$

where τ_s from Eq. (24) depends only on s, like $Z_s(E)$ that denotes the spin-resolved density of states; $\langle \epsilon_s^{-2} \rangle$ is the mean inverse-square band distance $E_{as\mathbf{k}} - E_{bs\mathbf{k}}$ measured from $E_{as\mathbf{k}} = E_F$ [as would be obtained from Eq. (25) with $|F|^2$ replaced by an average value], and $\langle \epsilon_s^{-1} \rangle$ is the analogously averaged inverse distance.

The second term in Eq. (28) is the correction to LTA, in this case definitely positive, but smaller than the LTA result because of dispersion in ϵ. Quantitative relevance of Eq. (28) is very small because the t_{2g} subspace used in the illustration contains only 20% of Tr $\mathbf{L}_j^2$ on each atom. Strict proportionality to $1/\tau$ results from neglecting $1/\tau^2$ in the Lorentzian denominators (12). However, the result may be extended to models with all five $3d$ bands; we have checked that the corrections computed numerically remain positive and smaller than the LTA result, which supports the relevance of the LTA for better than only qualitative estimates.

C. Numerical results

Correspondence of the intraband contributions to λ [$m=n$ in Eq. (14)], with the result derived previously from the model of "breathing" Fermi surface,[18,19] may be shown analytically. The squared Lorentzian in Eq. (14) gives $\pi/2w = \pi\tau$ on integration over $E'_{m\mathbf{k}}$ through its peak at $E'_{m\mathbf{k}}=0$; the peak is very sharp and selects the peak value of the squared matrix element, i.e., it has the same effect[45] as $\pi\tau\delta(E'_{m\mathbf{k}})$. The intraband contribution λ_D is, thus, proportional to the lifetime τ, with

$$\frac{\lambda_D}{\tau} = \frac{\gamma^2\hbar}{2\Omega_{at}} \left\langle \sum_{n\mathbf{k}} |F^{\dagger}_{n\mathbf{k},n\mathbf{k}}|^2 \delta(E'_{n\mathbf{k}}) \right\rangle_{\mathbf{k}} \tag{29}$$

(we recall that F and E' are assumed in frequency units).

The high λ in Ni at low values of $1/\tau$ correspond to the low-temperature FMR experiments pioneered by Rodbell.[3,6,8] The calculated values of λ_D/τ are 6.5×10^{21} s^{-2} for Ni and only 0.74×10^{21} s^{-2} for Fe (by an order of magnitude less), in fair agreement with the *ab initio* calculations.[18,19]

Tracking the origin of these high values in Ni shows that the diagonal effective-field elements $F^{+}_{m\mathbf{k},m\mathbf{k}}$ are large, of first

order in the SOC parameter ξ, on two large minority-spin sheets of the Fermi surface near their intersections with the {110} planes[46] (between the ΓX and ΓL symmetry axes), where the sheets are accidentally almost in contact. Diagonal elements of $\mathbf{L}$ and $F^{\pm}$ are restored by SOC wherever the strength of orbital momentum quenching, measured by the vertical splitting between the cubic band energies, is small. No such wide areas of nearby Fermi surface sheets are observed in Fe. The integral weight of the low-splitting areas near the symmetry degeneracies on the ⟨100⟩ axes in the $\mathbf{k}$ space (quoted in earlier qualitative considerations[21]) is relatively very small both in Fe and Ni.

The interband contributions to λ (dashed lines in Figs. 1 and 2) first increase in proportion to $1/\tau$. It corresponds qualitatively to $m \neq n$ terms in the formula

$$\lambda_{\mathrm{off}} \cong \frac{\gamma^2 \hbar}{\Omega_{at}} \left\langle \sum_{m \neq n} |F^{\dagger}_{m\mathbf{k},n\mathbf{k}}|^2 \frac{w}{\epsilon^2_{mn,\mathbf{k}} + 4w^2} \delta(E'_{n\mathbf{k}}) \right\rangle_{\mathbf{k}}, \quad (30)$$

with $\epsilon_{mn,\mathbf{k}} = E'_{m\mathbf{k}} - E'_{n\mathbf{k}}$. The form of Eq. (30) [obtainable analogously[45] to Eq. (29)] corresponds to intuitive broadening of the *transition* resonance in Eq. (8) rather than of the individual *levels* in Eq. (10). The initial increase of $\lambda_{\mathrm{off}} \propto 1/\tau$ occurs in the range of $2w = 1/\tau$ smaller than the minimum interband gaps, which arises from the SOC splitting of cubic degeneracies and are of the order of the SOC parameter ξ.

The flat parts of the λ vs $1/\tau$ plots at high $1/\tau$ result qualitatively from integration over the wide spectrum of the vertical interband intervals $\epsilon_{mn,\mathbf{k}}$ in Eq. (30). It corresponds to the flat part of the temperature dependence[6,7] of λ in Ni.

The computed values of λ are 0.36×10^8 s^{-1} at the minimum in Fe and 1.31×10^8 s^{-1} in the flat part in Ni, both about one-half of the experimental values.[6,7,9]

The nonvanishing damping with only weak dependence on the electron lifetime when $1/\tau$ exceeds the SOC parameter ξ was our main qualitative result.[21] It indicates chances to interpret quantitatively the relatively low damping observed in many high-resistivity alloys.

V. CONCLUDING REMARKS

Alternative derivations of formulas estimating the Gilbert damping coefficient in terms of earlier phenomenology of magnon-electron interaction[27] and from an extension of formal linear-response theory[21,24] may hopefully contribute to the general consensus on the importance of the interaction of uniform magnons with orbital moments of $3d$ electrons near the Fermi level.

Numerical results based on *ab initio* electron energy spectra confirm that it may account for a substantial part of the Gilbert damping in iron and nickel. The calculated damping is much higher in nickel than in iron, particularly at low electron scattering rates, in accordance with the model of breathing Fermi surface and with ferromagnetic resonance data. At higher scattering rates expected at room temperature and also in alloys, the calculated values are smaller than the experimental values by a factor of about 2 (but much higher than in the model of breathing Fermi surface). Since in this region they exhibit only very little dependence on the electron scattering rates, our ignorance about the scattering mechanisms is less prohibitive than it would be in the theory of resistivity.

The results of evaluation of the same formula (13) with Eq. (12) reported in Ref. 20 were published after submission of the present work; the values of λ in the regions of high $1/\tau$ are somewhat higher than our estimates (by approximately 10% in Fe and by approximately 20% in Ni).

The fact that the lifetime approximation (LTA) (13) neglects disorder in the spin-orbit coupling may be one reason why the calculated damping is smaller than the experimental data. The discussion of the relevance of the LTA in Sec. IV B and the model calculation of the vertex correction in Appendix B indicate that neglecting the correction may also lead to underestimated damping.

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APPENDIX A: LINEAR RESPONSE

Linear response to a harmonic field such that $h_x - ih_y$ is proportional to $e^{-i\omega t}$ is described by a single susceptibility function $\chi_m(\omega)$ if $\mathbf{z}$ is at least threefold axis of crystal symmetry. The drive field and the response are clockwise (CW) or counterclockwise (CCW) polarized depending on the sign of ω. The Gilbert equation predicts

$$\chi_m(\omega) = -\gamma M_s (\omega - \gamma H_{\mathrm{eff}} + i\alpha\omega)^{-1}. \quad (A1)$$

Proportionality between the magnetization and the total spin allows us to consider only the transverse spin susceptibility $\chi_s(\omega)$ determined by formal first-order response theory[34,35] as

$$\chi_s(\omega) = -i \int_0^{\infty} e^{i(\omega+i0)} \langle [S^-(t), S^+] \rangle_T, \quad (A2)$$

where $\langle\ \rangle_T$ denotes the average over the equilibrium density matrix and $S^-(t)$ denotes the Heisenberg time dependence, which may be written as $S^-(t) = \exp(-it\mathcal{H})S^-$, where

$$\mathcal{H}A = [A, H] \quad (A3)$$

denotes commutation with the Hamiltonian H divided by $\hbar$ (i.e., H in frequency units) for any operator A.

Korenman and Prange noticed[24] that the mean commutator in Eq. (A2) is a bilinear function in the Hilbert space of operators, with all properties of an inner product, except positive definiteness. It may be denoted as

$$\{A|B\} = \langle [B, A^{\dagger}] \rangle_T. \quad (A4)$$

Symbolic integration in Eq. (A2) shows that such definition allows us to write $\chi_s(\omega)$ as a diagonal matrix element

$$\chi_s(\omega) = \{S^-|\mathcal{G}(\omega + i0)S^-\} \tag{A5}$$

of the resolvent of the "superoperator" $\mathcal{H}$, satisfying

$$z\mathcal{G}(z) = 1 + \mathcal{H}\mathcal{G}(z) \tag{A6}$$

for complex z off the real axis. The diagonal elements of these three terms are

$$z\chi_s(z) = N_s + \{S^-|\mathcal{H}\mathcal{G}(z)S^-\}, \tag{A7}$$

with the same N_s as in Eq. (3). The last term may be factorized into a product with $\chi_s(z)$, in analogy to similar tasks in irreversible statistics.[36] Defining a projector $\mathcal{P}$ onto S^-, based on Eq. (A4), as

$$\mathcal{P}A = N_s^{-1}\{S^-|A\}S^-, \tag{A8}$$

we may separate $\mathcal{G}(z)$ in Eq. (A7) into $\mathcal{P}\mathcal{G}(z)$ and $\mathcal{Q}\mathcal{G}(z)$, where $\mathcal{Q}=1-\mathcal{P}$, and observe that

$$\mathcal{P}\mathcal{G}(z)S^- = N_s^{-1}\chi_s(z)S^-. \tag{A9}$$

To factorize similarly the other term, $\mathcal{Q}\mathcal{G}(z)S^-$, we need the modified resolvent

$$\mathcal{G}_Q(z) = \mathcal{Q}(z - \mathcal{H}\mathcal{Q})^{-1} \tag{A10}$$

describing excitations in the space of variables not proportional to the collective S^-. We get

$$\mathcal{Q}\mathcal{G}(z)S^- = N_s^{-1}\chi_s(z)\mathcal{G}_Q(z)\mathcal{H}S^- \tag{A11}$$

from Eq. (A6), written as $(z-\mathcal{H}\mathcal{Q})\mathcal{G}(z)=1+\mathcal{H}\mathcal{P}\mathcal{G}(z)$ and multiplied by $\mathcal{G}_Q$ from the left. Substituting Eqs. (A9) and (A11) into Eq. (A7) and observing that $\mathcal{H}$ is Hermitian in the product (A4), we get $\chi_s(z)$ in the required form

$$\chi_s(\omega) = N_s[z - \Lambda^o - \Lambda^m(\omega + i0)]^{-1}, \tag{A12a}$$

$$\Lambda^o = N_s^{-1}\{S^-|\mathcal{H}S^-\}, \tag{A12b}$$

$$\Lambda^m(z) = N_s^{-1}\{F^-|\mathcal{G}_Q(z)F^-\}, \tag{A12c}$$

$$F^- = \mathcal{H}S^-. \tag{A12d}$$

The real term Λ^o was identified by other authors.[24] The real part of self-energy [corresponding to $\gamma H_{\rm eff}$ in Eq. (A1)] needs *both* Eq. (A12b) and the real part of Eq. (A12c); both these terms are of order ξ^2, but their balance is of order ξ^4 in cubic crystals,[47] as in the static theory.[12]

The complex Λ^m contains the damping in the imaginary part. Comparing Eqs. (A1) and (A12a) gives

$$\alpha(\omega) = -\omega^{-1}\,\mathrm{Im}\,\Lambda^m(\omega + i0). \tag{A13}$$

Obtaining Eq. (9) form Eq. (A13) requires the following additional steps: (i) replacing $\mathcal{G}_Q$ in Eq. (A12c) by $\mathcal{G}_{\rm mf}$ from Eq. (A6), with $\mathcal{H}=\mathcal{H}_{\rm mf}$ consisting of electron transition frequencies in mean-field approximation, and (ii) adiabatic approximation for the general average of one-electron variables, $\langle A\rangle_T=\langle \mathrm{Tr}[f(H_{\rm mf})A]\rangle_c$, where $f(E)$ is the Fermi function and $\langle\ \rangle_c$ denotes configuration average added for the lattice degrees of freedom. Then $\mathcal{H}_{\rm mf}$ may be at least symbolically diagonalized as $\mathcal{H}_{\mu\nu,\mu\nu}=E_\nu-E_\mu$, and Eq. (9) follows from Eq. (A13) with $\mathrm{Im}(E+i0)=-\pi\delta(E)$ in the limit of $\omega\to 0$.

The projection formalism allows us to use the mean-field approximation only for the low-frequency self-energy (rather than for the spin susceptibility, where it would be hardly appropriate). The mean-field approximation is used for the low-frequency dynamics of the effective fields, and particularly for the damping term determined by electron spectra near the Fermi level. Formal separation of the effective-field modes from the collective magnon corresponds to the intuitive form of the magnon-electron interaction (2).

APPENDIX B: WEAK SCATTERING

Perturbation theory for the Lorentzian mean spectral densities and consistently averaged $\langle DFD\rangle_c$ products needed in linear response is reviewed, e.g., by Velický.[48] The resolvent $G(z)=(z-H_0-V)^{-1}$, where H_0 is periodic and V is random, determines both from

$$D(E) = \frac{i}{2\pi}\sum_{t=\pm 1} tG(E^t), \tag{B1}$$

$$\langle D(E)FD(E)\rangle_c = \frac{-1}{4\pi^2}\sum_{t,t'=\pm 1} tt'K(E^t,E^{t'}), \tag{B2}$$

$$K(z_1,z_2) = \langle G(z_1)FG(z_2)\rangle_c, \tag{B3}$$

with $E^t=E+it\epsilon$, $\epsilon\to 0+$, and $F=F^-$ for brevity. The average

$$\bar{G}(z) = \langle G(z)\rangle_c = [z - H_0 - \sigma(z)]^{-1} \tag{B4}$$

defines the complex self-energy $\sigma(z)$, which distinguishes the average propagator $\bar{G}$ from the unperturbed $G_0=(z-H_0)^{-1}$. The average $\langle D(E)\rangle_c$ from Eq. (B1) has the form (12) with $\mathrm{Re}\,\sigma_{m\mathbf{k}}(E^-)$ added to $E_{m\mathbf{k}}(E^-)$ and

$$w_{m\mathbf{k}} = \mathrm{Im}\,\sigma_{m\mathbf{k}}(E^-). \tag{B5}$$

Iteration to order V^2 in the *second* line of the well-known identities

$$G = G_0 + G_0VG \tag{B6a}$$

$$= \bar{G} + \bar{G}(V-\sigma)G \tag{B6b}$$

gives

$$\sigma(z) = \langle V\bar{G}(z)V\rangle_c, \tag{B7}$$

$$K(z_1,z_2) = \bar{G}(z_1)[F + \langle VK^{(L)}V\rangle_c]\bar{G}(z_2), \tag{B8}$$

$$K^L(z_1,z_2) = \bar{G}(z_1)F\bar{G}(z_2). \tag{B9}$$

Using $\bar{G}$ instead of G_0 in these expansions removes the inconsistency of sharp energy levels in the simpler approximations based on Eq. (22).

While $K^{(L)}$ alone gives the lifetime approximation, the term $\langle VKV\rangle_c$ in Eq. (B8) appears as a correction to F interaction (called, therefore, vertex correction).

Application of this general expansion is very simple in the model used in the qualitative theories of magnetic anisotropy[12] and nuclear spin relaxation,[41] with Bloch states of the LCAO form (21) with definite spin and the AO restricted to the three t_{2g} functions. Recalling the definition of the single-site F_j elements in Eqs. (6) and (5b), we may write Eq. (B9) in the AO representation as

$$\hat{K}_j^{(L)ss'} = \sum_i \hat{\bar{G}}_{ji}^{s} \hat{F}_i^{ss'} \hat{\bar{G}}_{ij}^{s'}, \tag{B10}$$

where hats denote matrices in the AO indices (α). As long as $\hat{F}_i$ is the same at all sites, so is $\hat{K}_j^{(L)}$, and the dyadic operation $\Sigma_i \hat{\bar{G}}_{ji}^{s} \ldots \hat{\bar{G}}_{ij}^{s'}$ exhibits cubic symmetry. Symmetrization may use the inverse transform from Eq. (21) to local AO, regarding that $\Sigma_i \hat{\bar{G}}_{ji}^{s} \ldots \hat{\bar{G}}_{ij}^{s'}$ is applied to the transfer of axial-vector variables[41] L^r. Summation of products containing four coefficients $C_{as\mathbf{k}}^{\alpha}$ over the cubic star of $\mathbf{k}$ then selects only one appropriate invariant and gives a simple result for the six-band t_{2g} model:

$$\hat{K}_j^{(L)ss'} = \hat{F}_j^{ss'} \cdot b_{ss'}, \tag{B11}$$

$$b_{ss'}(z_1,z_2) = \frac{1}{N_{at}} \sum_{\mathbf{k},a\neq b} \bar{G}_{as\mathbf{k}}(z_1) \bar{G}_{bs'\mathbf{k}}(z_2). \tag{B12}$$

Substitution to Eqs. (B9), (B2), and (10b) gives the LTA,

$$\alpha_E^{(L)} = \frac{\pi\xi^2}{6N_s} \sum_{\mathbf{k},a\neq b,s,s'} \bar{D}(E)_{as\mathbf{k}} \bar{D}(E)_{bs'\mathbf{k}}, \tag{B13}$$

where $\bar{D}_{as\mathbf{k}} = \langle D_{as\mathbf{k}} \rangle_c$ has the form (12), with $w_{as\mathbf{k}}$ from Eq. (B5) and the local symmetrized $\mathrm{Tr}(\hat{F}_j^{+ss'} \hat{F}_j^{s's} + \hat{F}_j^{+s's} \hat{F}_j^{ss'})$ equal to $2\xi^2$ in the t_{2g} model. Equation (B13) also follows from Eq. (13), with the interband $|F^{+}_{as\mathbf{k},bs'\mathbf{k}}|^2$ replaced by the cubic average $\xi^2/6$ in the t_{2g} model.

Disorder may simply be modeled by point defects at random sites i,

$$V = \sum_{i,\alpha} v_i |\alpha i\rangle\langle \alpha i|, \tag{B14}$$

with no effect on the AO shapes, and random changes of $\mathbf{k}$ of the band states taken into account by single-site averages in $\langle\ \rangle_c$. Then the self-energy (at $E=E_F$) in the t_{2g} model depends only on the spin, with

$$w_s = (2\tau_s)^{-1} = (\pi/3) v^2 Z_s(E), \tag{B15}$$

where $Z_s(E)$ is the spin-resolved density of states (per atom) and $v^2 = \langle v_i^2 \rangle_c$.

The result for the vertex correction in Eq. (B8) written in local representation is also simple: the mean local $\langle V \hat{K}_j^{(L)} V \rangle_c$ equals $v^2 \hat{K}_j^{(L)}$ and the second term in Eq. (B8) is

$$\hat{K}_j^{(V)ss'} = \hat{F}_j^{ss'} \cdot v^2 b_{ss'}^2. \tag{B16}$$

Substitution to Eqs. (B8), (B2), and (10b) gives additional terms to α_E, i.e., the correction to the LTA,

$$\alpha_E^{(V)} = \frac{\pi\xi^2}{N_{s/\mathrm{at}}} 2v^2\, \mathrm{Tr}(PP^{\dagger}), \tag{B17}$$

where $N_{s/at} = N_s/N_{at}$, and P is a 2×2 matrix in s,

$$P_{ss'} = \frac{1}{6N_{at}} \sum_{\mathbf{k},a\neq b} \bar{D}_{as\mathbf{k}}\, \mathrm{Re}\, \bar{G}_{bs'\mathbf{k}}. \tag{B18}$$

Equation (28) is obtained if $\bar{D}$ in Eq. (B13), and Eq. (B18) is approximated as in Eq. (26) and $\mathrm{Re}\, \bar{G}_{as\mathbf{k}}$ as $(E-E_{as\mathbf{k}})^{-1}$. The products $P_{ss'}P_{s's}$ are obviously positive for $s=s'$, indicating that the vertex correction in this model would enhance the LTA value of the damping parameter. Numerical results obtained with this scattering model and including all $3d$ bands (and scalar $b_{ss'}$ replaced by 3×3 matrices) confirmed this conclusion.

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