Gilbert damping in conducting ferromagnets. I. Kohn-Sham theory and atomic-scale inhomogeneity

Ion Garate and Allan MacDonald
Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA
(Received 9 August 2008; revised manuscript received 13 September 2008; published 5 February 2009)

We derive an approximate expression for the Gilbert damping coefficient α_G of itinerant electron ferromagnets which is based on their description in terms of spin-density-functional theory (SDFT) and Kohn-Sham quasiparticle orbitals. We argue for an expression in which the coupling of magnetization fluctuations to particle-hole transitions is weighted by the spin-dependent part of the theory's exchange-correlation potential, a quantity which has large spatial variations on an atomic length scale. Our SDFT result for α_G is closely related to the previously proposed spin-torque correlation-function expression.

DOI: 10.1103/PhysRevB.79.064403 PACS number(s): 76.20.+q

I. INTRODUCTION

The Gilbert parameter α_G characterizes the damping of collective magnetization dynamics.[1] The key role of α_G in current-driven[2] and precessional[3] magnetization reversals has renewed interest in the microscopic physics of this important material parameter. It is generally accepted that in metals the damping of magnetization dynamics is dominated[3] by particle-hole pair excitation processes. The main ideas which arise in the theory of Gilbert damping have been in place for some time.[4,5] It has however been difficult to apply them to real materials with the precision required for confident predictions which would allow theory to play a larger role in designing materials with desired damping strengths. Progress has recently been achieved in various directions, both through studies[6] of simple models for which the damping can be evaluated exactly and through analyses[7–9] of transition-metal ferromagnets that are based on realistic electronic structure calculations. Evaluation of the torque-correlation formula[8,9] for α_G used in the later calculations requires knowledge only of a ferromagnet's mean-field electronic structure and of its Bloch state lifetime, which makes this approach practical.

Realistic *ab initio* theories normally employ spin-density-functional theory[10] which has a mean-field theory structure. In this paper we use time-dependent spin-density-functional theory[11] to derive an explicit expression for the Gilbert damping coefficient in terms of Kohn-Sham theory eigenvalues and eigenvectors. Our final result is essentially equivalent to the torque-correlation formula[5] for α_G, but has the advantages that its derivation is fully consistent with density-functional theory, that it allows for a consistent microscopic treatments of both dissipative and reactive coefficients in the Landau-Liftshitz-Gilbert (LLG) equations and that it helps establish relationships between different theoretical approaches to the microscopic theory of magnetization damping.

Our paper is organized as follows. In Sec. II we relate the Gilbert damping parameter α_G of a ferromagnet to the low-frequency limit of its transverse-spin-response function. Since ferromagnetism is due to electron-electron interactions, theories of magnetism are always many-electron theories and it is necessary to evaluate the many-electron response function. In time-dependent spin-density-functional theory the transverse response function is calculated using a time-dependent self-consistent-field calculation in which quasiparticles respond both to external potentials and to changes in the interaction-induced effective potential. In Sec. III we use perturbation theory and time-dependent mean-field theory to express the coefficients which appear in the LLG equations in terms of the Kohn-Sham eigenstates and eigenvalues of the ferromagnet's ground state. These formal expressions are valid for arbitrary spin-orbit coupling, arbitrary atomic length scale spin-dependent and scalar potentials, and arbitrary disorder. By treating disorder approximately, in Sec. IV we derive and compare two commonly used formulas for Gilbert damping. Finally, in Sec. V we summarize our results.

This is the first of two papers related to damping of collective magnetization dynamics in metallic ferromagnets. The second paper will report on *exact* calculations for two different toy-model systems, with and without intrinsic spin-orbit interactions and with various spin-independent and spin-dependent disorder models. These model calculations shed light on the absolute and relative reliabilities of the two different formulas for α_G discussed in the present paper. Paper II will additionally highlight the importance of higher order diffusive particle-hole correlations in strongly spin-orbit coupled systems such as (Ga,Mn)As.

II. MANY-BODY TRANSVERSE RESPONSE FUNCTION AND THE GILBERT DAMPING PARAMETER

The Gilbert damping parameter α_G appears in the Landau-Liftshitz-Gilbert expression for the collective magnetization dynamics of a ferromagnet

$$\frac{\partial \hat{\Omega}}{\partial t} = \hat{\Omega} \times \mathcal{H}_{\text{eff}} - \alpha_G \hat{\Omega} \times \frac{\partial \hat{\Omega}}{\partial t}. \tag{1}$$

In Eq. (1) $\mathcal{H}_{\text{eff}}$ is an effective magnetic field which we comment on further below and $\hat{\Omega} \simeq [\Omega_x, \Omega_y, 1-(\Omega_x^2+\Omega_y^2)/2]$ is the direction of the magnetization.[12] This equation describes the slow dynamics of smooth magnetization textures and is formally the first term in an expansion in time derivatives.

The damping parameter α_G can be measured by performing ferromagnetic resonance (FMR) experiments in which the magnetization direction is driven weakly away from an easy direction (which we take to be the $\hat{z}$ direction). To relate this phenomenological expression formally to microscopic theory we consider a system in which external magnetic fields couple only[13] to the electronic spin degree of freedom and associate the magnetization direction $\hat{\Omega}$ with the direction of the total electron spin. For small deviations from the easy direction, Eq. (1) reads

$$\mathcal{H}_{\mathrm{eff},x} = +\frac{\partial \hat{\Omega}_y}{\partial t} + \alpha_G \frac{\partial \hat{\Omega}_x}{\partial t},$$

$$\mathcal{H}_{\mathrm{eff},y} = -\frac{\partial \hat{\Omega}_x}{\partial t} + \alpha_G \frac{\partial \hat{\Omega}_y}{\partial t}. \tag{2}$$

The gyromagnetic ratio has been absorbed into the units of the field $\mathcal{H}_{\mathrm{eff}}$ so that this quantity has energy units and we set $\hbar = 1$ throughout. The corresponding formal linear-response theory expression is an expansion of the long-wavelength transverse total spin-response function to first order[14] in frequency ω,

$$S_0 \hat{\Omega}_\alpha = \sum_\beta [\chi^{\mathrm{st}}_{\alpha,\beta} + \omega \chi'_{\alpha,\beta}] \mathcal{H}_{\mathrm{ext},\beta}, \tag{3}$$

where $\alpha, \beta \in \{x, y\}$, $\omega \equiv i\partial_t$ is the frequency, S_0 is the total spin of the ferromagnet, $\mathcal{H}_{\mathrm{ext}}$ is the external magnetic field, and χ is the transverse spin-spin response function

$$\begin{aligned}\chi_{\alpha,\beta}(\omega) &= i\int_0^\infty dt\, \exp(i\omega t)\langle [S_\alpha(t), S_\beta(0)]\rangle \\ &= \sum_n \left[\frac{\langle \Psi_0|S_\alpha|\Psi_n\rangle\langle \Psi_n|S_\beta|\Psi_0\rangle}{\omega_{n,0} - \omega - i\eta} \right. \\ &\quad \left. + \frac{\langle \Psi_0|S_\beta|\Psi_n\rangle\langle \Psi_n|S_\alpha|\Psi_0\rangle}{\omega_{n,0} + \omega + i\eta} \right],\end{aligned} \tag{4}$$

Here $|\Psi_n\rangle$ is an exact eigenstate of the many-body Hamiltonian and $\omega_{n,0}$ is the excitation energy for state n. We use this formal expression below to make some general comments about the microscopic theory of α_G. In Eq. (3) $\chi^{\mathrm{st}}_{\alpha,\beta}$ is the static ($\omega = 0$) limit of the response function and $\chi'_{\alpha,\beta}$ is the first derivative with respect to ω evaluated at $\omega = 0$. Notice that we have chosen the normalization in which χ is the total spin response to a transverse field; χ is therefore extensive.

The key step in obtaining the Landau-Liftshitz-Gilbert form for the magnetization dynamics is to recognize that in the static limit the transverse magnetization responds to an external magnetic field by adjusting orientation to minimize the total energy including the internal energy E_{int} and the energy due to coupling with the external magnetic field

$$E_{\mathrm{ext}} = -S_0 \hat{\Omega} \cdot \mathcal{H}_{\mathrm{ext}}. \tag{5}$$

It follows that

$$\chi^{\mathrm{st}}_{\alpha,\beta} = S_0^2 \left[\frac{\partial^2 E_{\mathrm{int}}}{\partial \hat{\Omega}_\alpha \partial \hat{\Omega}_\beta} \right]^{-1}. \tag{6}$$

We obtain a formal equation for H_{eff} corresponding to Eq. (2) by multiplying Eq. (3) on the left by $[\chi^{\mathrm{st}}_{\alpha,\beta}]^{-1}$ and recognizing

$$\mathcal{H}_{\mathrm{int},\alpha} = -\frac{1}{S_0} \sum_\beta \frac{\partial^2 E_{\mathrm{int}}}{\partial \hat{\Omega}_\alpha \partial \hat{\Omega}_\beta} \hat{\Omega}_\beta = -\frac{1}{S_0} \frac{\partial E_{\mathrm{int}}}{\partial \hat{\Omega}_\alpha} \tag{7}$$

as the internal energy contribution to the effective magnetic field $\mathcal{H}_{\mathrm{eff}} = \mathcal{H}_{\mathrm{int}} + \mathcal{H}_{\mathrm{ext}}$. With this identification Eq. (3) can be written in the form

$$H_{\mathrm{eff},\alpha} = \sum_\beta \mathcal{L}_{\alpha,\beta} \partial_t \hat{\Omega}_\beta, \tag{8}$$

where

$$\mathcal{L}_{\alpha,\beta} = -S_0 [i(\chi^{\mathrm{st}})^{-1} \chi' (\chi^{\mathrm{st}})^{-1}]_{\alpha,\beta} = i S_0 \partial_\omega \chi^{-1}_{\alpha,\beta}. \tag{9}$$

According to the Landau-Liftshitz-Gilbert equation then $\mathcal{L}_{x,y} = -\mathcal{L}_{y,x} = 1$ and

$$\mathcal{L}_{x,x} = \mathcal{L}_{y,y} = \alpha_G. \tag{10}$$

Explicit evaluation of the off-diagonal components of $\mathcal{L}$ will in general yield very small deviation from the unit result assumed by the Landau-Liftshitz-Gilbert formula. The deviation reflects mainly the fact that the magnetization magnitude varies slightly with orientation. We do not comment further on this point because it is of little consequence. Similarly $\mathcal{L}_{x,x}$ is not in general identical to $\mathcal{L}_{y,y}$, although the difference is rarely large or important when the magnetization is aligned with a high-symmetry direction of a hexagonal or cubic crystal.[7] Equation (10) is the starting point we use later to derive approximate expressions for α_G.

In Eq. (9) $\chi_{\alpha,\beta}(\omega)$ is the correlation function for an interacting electron system with arbitrary disorder and arbitrary spin-orbit coupling. In the absence of spin-orbit coupling, but still with arbitrary spin-independent periodic and disorder potentials, the ground state of a ferromagnet is coupled by the total spin-operator only to states in the same total spin multiplet. In this case it follows from Eq. (4) that

$$\chi^{\mathrm{st}}_{\alpha,\beta} = 2\sum_n \frac{\mathrm{Re}[\langle \Psi_0|S_\alpha|\Psi_n\rangle\langle \Psi_n|S_\beta|\Psi_0\rangle]}{\omega_{n,0}} = \delta_{\alpha,\beta} \frac{S_0}{H_0}, \tag{11}$$

where H_0 is a static external field, which is necessary in the absence of spin-orbit coupling to pin the magnetization to the $\hat{z}$ direction and splits the ferromagnet's ground-state many-body spin multiplet. Similarly

$$\chi'_{\alpha,\beta} = 2i\sum_n \frac{\mathrm{Im}[\langle \Psi_0|S_\alpha|\Psi_n\rangle\langle \Psi_n|S_\beta|\Psi_0\rangle]}{\omega^2_{n,0}} = i\epsilon_{\alpha,\beta} \frac{S_0}{H_0^2}, \tag{12}$$

where $\epsilon_{x,x} = \epsilon_{y,y} = 0$ and $\epsilon_{x,y} = -\epsilon_{y,x} = 1$, yielding $\mathcal{L}_{x,y} = -\mathcal{L}_{y,x} = 1$ and $\mathcal{L}_{x,x} = \mathcal{L}_{y,y} = 0$. Spin-orbit coupling is required for magnetization damping.[15]

III. SDF-STONER THEORY EXPRESSION FOR GILBERT DAMPING

Approximate formulas for α_G in metals are inevitably based on a self-consistent mean-field theory (Stoner) description of the magnetic state. Our goal is to derive an approximate expression for α_G when the adiabatic local spin-density approximation[10] is used for the exchange-correlation potential in spin-density-functional theory. The effective Hamiltonian which describes the Kohn-Sham quasiparticle dynamics therefore has the form

$$\mathcal{H}_{\mathrm{KS}} = \mathcal{H}_P - \Delta[n(\vec{r}),|\vec{s}(\vec{r})|]\hat{\Omega}(\vec{r})\cdot\vec{s}, \tag{13}$$

where $\mathcal{H}_P$ is the Kohn-Sham Hamiltonian of a paramagnetic state in which $|\vec{s}(\vec{r})|$(the local spin density) is set to zero, $\vec{s}$ is the spin-operator, and

$$\Delta(n,s) = -\frac{d[n\epsilon_{\mathrm{xc}}(n,s)]}{ds} \tag{14}$$

is the magnitude of the spin-dependent part of the exchange-correlation potential. In Eq. (14) $\epsilon_{\mathrm{xc}}(n,s)$ is the exchange-correlation energy per particle in a uniform electron gas with density n and spin-density s. We assume that the ferromagnet is described using some semirelativistic approximation to the Dirac equation such as those commonly used[16] to describe magnetic anisotropy or x-ray magnetic circular dichroism, even though these approximations are not strictly consistent with spin-density-functional theory. Within this framework electrons carry only a two-component spin-1/2 degree of freedom and spin-orbit coupling terms are included in $\mathcal{H}_P$. Since $n\epsilon_{\mathrm{xc}}(n,s)\sim[(n/2+s)^{4/3}+(n/2-s)^{4/3}]$, $\Delta(n,s)\sim n^{1/3}$ is larger closer to atomic centers and far from spatially uniform on atomic length scales.[17] This property figures prominently in the considerations explained below.

In spin-density-functional theory (SDFT) the transverse-spin-response function is expressed in terms of Kohn-Sham quasiparticle response to both external and induced magnetic fields

$$s_0(\vec{r})\Omega_\alpha(\vec{r}) = \int \frac{d\vec{r}'}{V}\chi^{\mathrm{QP}}_{\alpha,\beta}(\vec{r},\vec{r}')[\mathcal{H}_{\mathrm{ext},\beta}(\vec{r}') + \Delta(\vec{r}')\Omega_\beta(\vec{r}')]. \tag{15}$$

In Eq. (15) V is the system volume, $s_0(\vec{r})$ is the magnitude of the ground-state spin density, $\Delta(\vec{r})$ is the magnitude of the spin-dependent part of the ground-state exchange-correlation potential, and

$$\chi^{\mathrm{QP}}_{\alpha,\beta}(\vec{r},\vec{r}') = \sum_{i,j}\frac{f_j - f_i}{\omega_{i,j} - \omega - i\eta}\langle i|\vec{r}\rangle s_\alpha\langle\vec{r}|j\rangle\langle j|\vec{r}'\rangle s_\beta\langle\vec{r}'|i\rangle, \tag{16}$$

where f_i is the ground-state Kohn-Sham occupation factor for eigenspinor $|i\rangle$ and $\omega_{ij}\equiv\epsilon_i-\epsilon_j$ is a Kohn-Sham eigenvalue difference. $\chi^{\mathrm{QP}}(\vec{r},\vec{r}')$ has been normalized so that it returns the spin-density rather than total spin. Like the Landau-Liftshitz-Gilbert equation itself, Eq. (15) assumes that only the direction of the magnetization, and not the magnitudes of the charge and spin-densities, varies in the course of smooth collective magnetization dynamics.[18] This property should hold accurately as long as magnetic anisotropies and external fields are weak compared to Δ. We are able to use this property to avoid solving the position-space integral equation implied by Eq. (15). Multiplying by $\Delta(\vec{r})$ on both sides and integrating over position we find[19] that

$$S_0\Omega_\alpha = \sum_\beta \frac{1}{\bar{\Delta}}\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}(\omega)\left[\Omega_\beta + \frac{\mathcal{H}_{\mathrm{ext},\beta}}{\bar{\Delta}}\right], \tag{17}$$

where we have taken advantage of the fact that in FMR experiments $\mathcal{H}_{\mathrm{ext},\beta}$ and $\hat{\Omega}$ are uniform. $\bar{\Delta}$ is a spin-density weighted average of $\Delta(\vec{r})$,

$$\bar{\Delta} = \frac{\int d\vec{r}\Delta(\vec{r})s_0(\vec{r})}{\int d\vec{r}s_0(\vec{r})}, \tag{18}$$

and

$$\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}(\omega) = \sum_{ij}\frac{f_j - f_i}{\omega_{ij} - \omega - i\eta}\langle j|s_\alpha\Delta(\vec{r})|i\rangle\langle i|s_\beta\Delta(\vec{r})|j\rangle \tag{19}$$

is the transverse part of the quasiparticle exchange-correlation effective-field response function, *not* the transverse part of the quasiparticle spin-response function. In Eq. (19), $\langle i|O(\vec{r})|j\rangle = \int d\vec{r}\langle i|\vec{r}\rangle O(\vec{r})\langle\vec{r}|j\rangle$ denotes a single-particle matrix element. Solving Eq. (17) for the many-particle transverse susceptibility (the ratio of $S_0\hat{\Omega}_\alpha$ to $H_{\mathrm{ext},\beta}$) and inserting the result in Eq. (9) yields

$$\mathcal{L}_{\alpha,\beta} = iS_0\partial_\omega\chi^{-1}_{\alpha,\beta} = -S_0\bar{\Delta}^2\partial_\omega\,\mathrm{Im}[\tilde{\chi}^{\mathrm{QP}-1}_{\alpha,\beta}]. \tag{20}$$

Our microscopic theory of the LLG damping parameter helps explain the relationship between a variety of similar but distinct formulas which appear in the literature in either *ab initio* theory or model calculations. As we have explained, α_G is fundamentally related to the full many-body transverse-spin-response function to smooth external magnetic fields. In SDFT and other theories with a similar mean-field structure, this translates not into the transverse-spin-response function of quasiparticles but instead into the quasiparticle response function for changes in the orientation of the spin-dependent part of the exchange-correlation potential. Spin-flip operators in this response function are therefore weighted by the local spin-splitting which varies considerably within each unit cell of a magnetic metal. In our formulation, as in some others[7] both reactive and dissipative terms in the LLG equation are understood in a consistent fashion. In addition, as we discuss in greater detail later, our approach treats the breathing Fermi-surface contribution to damping[5,7] and the interband spin-relaxation contribution on the same footing. Using our formulation we are able below to address the relationship between torque-correlation formulas for the magnetization damping and other spin-oriented formulas which arise more naturally in Kubo response function theories for model systems.

Comparing Eqs. (7) and (15) we find that the internal anisotropy field can also be expressed in terms of $\tilde{\chi}^{\mathrm{QP}}$,

$$\mathcal{H}_{\mathrm{int},\alpha} = -\bar{\Delta}^2 S_0 \sum_\beta \left[\tilde{\chi}^{\mathrm{QP}-1}_{\alpha,\beta}(\omega=0) - \frac{\delta_{\alpha,\beta}}{S_0 \bar{\Delta}} \right] \Omega_\beta. \quad (21)$$

Equations (20) and (21) provide microscopic expressions for all ingredients that appear in the LLG equations linearized for small transverse excursions. It is generally assumed that the damping coefficient α_G is independent of orientation; if so, the present derivation is sufficient. The anisotropy field at large transverse excursions normally requires additional information about magnetic anisotropy. We remark that if the Hamiltonian does not include a spin-dependent mean-field dipole interaction term, as is usually the case, the above quantity will return only the magnetocrystalline anisotropy field. Since the magnetostatic contribution to anisotropy is always well described by mean-field theory it can be added separately.

We conclude this section by demonstrating that the Stoner-theory equations proposed here recover the exact results mentioned at the end of Sec. II for the limit in which spin-orbit coupling is neglected. We consider a SDFT ferromagnet with arbitrary scalar and spin-dependent effective potentials. Since the spin-dependent part of the exchange-correlation potential is then the only spin-dependent term in the Hamiltonian it follows that

$$[\mathcal{H}_{\mathrm{KS}}, s_\alpha] = -i\epsilon_{\alpha,\beta}\Delta(\vec{r}) s_\beta \quad (22)$$

and hence that

$$\langle i|s_\alpha \Delta(\vec{r})|j\rangle = -i\epsilon_{\alpha,\beta}\omega_{ij}\langle i|s_\beta|j\rangle. \quad (23)$$

Inserting Eq. (23) in one of the matrix elements of Eq. (19) yields for the no-spin-orbit-scattering case

$$\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}(\omega=0) = \delta_{\alpha,\beta} S_0 \bar{\Delta}. \quad (24)$$

The internal magnetic field $\mathcal{H}_{\mathrm{int},\alpha}$ is therefore identically zero in the absence of spin-orbit coupling and only external magnetic fields will yield a finite collective precession frequency. Inserting Eq. (23) in both matrix elements of Eq. (19) yields

$$\partial_\omega \,\mathrm{Im}[\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}] = \epsilon_{\alpha,\beta} S_0. \quad (25)$$

Using both Eqs. (24) and (25) to invert $\tilde{\chi}^{\mathrm{QP}}$ we recover the results proved previously for the no-spin-orbit case using a many-body argument: $\mathcal{L}_{x,y}=-\mathcal{L}_{y,x}=1$ and $\mathcal{L}_{x,x}=\mathcal{L}_{y,y}=0$. The Stoner-theory equations derived here allow spin-orbit interactions, and hence magnetic anisotropy and Gilbert damping, to be calculated consistently from the same quasiparticle response function $\tilde{\chi}^{\mathrm{QP}}$.

IV. DISCUSSION

As long as magnetic anisotropy and external magnetic fields are weak compared to the exchange-correlation splitting in the ferromagnet we can use Eq. (24) to approximate $\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}(\omega=0)$. Using this approximation and assuming that damping is isotropic we obtain the following explicit expression for temperature $T\to 0$:

$$\begin{aligned}\alpha_G = \mathcal{L}_{x,x} &= -S_0\bar{\Delta}^2 \partial_\omega \,\mathrm{Im}[\tilde{\chi}^{\mathrm{QP}-1}_{x,x}] \\ &= \frac{\pi}{S_0}\sum_{ij} \delta(\epsilon_j-\epsilon_F)\delta(\epsilon_i-\epsilon_F)\langle j|s_x\Delta(\vec{r})|i\rangle\langle i|s_x\Delta(\vec{r})|j\rangle \\ &= \frac{\pi}{S_0}\sum_{ij} \delta(\epsilon_j-\epsilon_F)\delta(\epsilon_i-\epsilon_F) \\ &\quad \times\langle j|[\mathcal{H}_P, s_y]|i\rangle\langle i|[\mathcal{H}_P, s_y]|j\rangle. \end{aligned} \quad (26)$$

The second form for α_G is equivalent to the first and follows from the observation that for matrix elements between states that have the same energy

$$\begin{aligned}\langle i|[\mathcal{H}_{\mathrm{KS}}, s_\alpha]|j\rangle &= -i\epsilon_{\alpha,\beta}\langle i|\Delta(\vec{r})s_\beta|j\rangle + \langle i|[\mathcal{H}_P, s_\alpha]|j\rangle \\ &= 0 \quad (\text{for } \omega_{ij}=0). \end{aligned} \quad (27)$$

Equation (26) is valid for any scalar and any spin-dependent potential. It is clear however that the numerical value of α_G in a metal is very sensitive to the degree of disorder in its lattice. To see this we observe that for a perfect crystal the Kohn-Sham eigenstates are Bloch states. Since the operator $\Delta(\vec{r})s_\alpha$ has the periodicity of the crystal its matrix elements are nonzero only between states with the same Bloch wave vector label $\vec{k}$. For the case of a perfect crystal then

$$\begin{aligned}\alpha_G &= \frac{\pi}{s_0}\int_{\mathrm{BZ}} \frac{d\vec{k}}{(2\pi)^3}\sum_{nn'} \delta(\epsilon_{\vec{k}n'}-\epsilon_F)\delta(\epsilon_{\vec{k}n}-\epsilon_F) \\ &\quad \times\langle \vec{k}n'|s_x\Delta(\vec{r})|\vec{k}n\rangle\langle\vec{k}n|s_x\Delta(\vec{r})|\vec{k}n'\rangle \\ &= \frac{\pi}{s_0}\int_{\mathrm{BZ}} \frac{d\vec{k}}{(2\pi)^3}\sum_{nn'} \delta(\epsilon_{\vec{k}n'}-\epsilon_F)\delta(\epsilon_{\vec{k}n}-\epsilon_F) \\ &\quad \times\langle \vec{k}n'|[\mathcal{H}_P, s_y]|\vec{k}n\rangle\langle\vec{k}n|[\mathcal{H}_P, s_y]|\vec{k}n'\rangle, \end{aligned} \quad (28)$$

where nn' are band labels and s_0 is the ground-state spin per unit volume and the integral over $\vec{k}$ is over the Brillouin zone (BZ).

Clearly α_G diverges[20] in a perfect crystal since $\langle\vec{k}n|s_x\Delta(\vec{r})|\vec{k}n\rangle$ is generically nonzero. A theory of α_G must therefore always account for disorder in a crystal.[21] The easiest way to account for disorder is to replace the $\delta(\epsilon_{\vec{k}n}-\epsilon_F)$ spectral function of a Bloch state by a broadened spectral function evaluated at the Fermi energy $A_{\vec{k}n}(\epsilon_F)$. If disorder is treated perturbatively this simple *ansatz* can be augmented[22] by introducing impurity vertex corrections in Eq. (28). Provided that the quasiparticle lifetime is computed via Fermi's golden rule, these vertex corrections restore Ward identities and yield an exact treatment of disorder in the limit of dilute impurities. Nevertheless, this approach is rarely practical outside the realm of toy models because the sources of disorder are rarely known with sufficient precision.

Although appealing in its simplicity, the $\delta(\epsilon_{\vec{k}n}-\epsilon_F) \to A_{\vec{k}n}(\epsilon_F)$ substitution is prone to ambiguity because it gives rise to qualitatively different outcomes depending on whether it is applied to the first or second line of Eq. (28)

$$\alpha_G^{(\mathrm{TC})} = \frac{\pi}{s_0}\int_{\mathrm{BZ}} \frac{d\vec{k}}{(2\pi)^3}\sum_{nn'} A_{\vec{k},n}(\epsilon_F)A_{\vec{k},n'}(\epsilon_F)\langle \vec{k}n'|[\mathcal{H}_P, s_y]|\vec{k}n\rangle \times \langle \vec{k}n|[\mathcal{H}_P, s_y]|\vec{k}n'\rangle,$$

$$\alpha_G^{(\mathrm{SF})} = \frac{\pi}{s_0}\int_{\mathrm{BZ}} \frac{d\vec{k}}{(2\pi)^3}\sum_{nn'} A_{\vec{k},n}(\epsilon_F)A_{\vec{k},n'}(\epsilon_F)\langle \vec{k}n'|s_x\Delta(\vec{r})|\vec{k}n\rangle \times \langle \vec{k}n|s_x\Delta(\vec{r})|\vec{k}n'\rangle. \quad (29)$$

$\alpha_G^{(\mathrm{TC})}$ is the torque-correlation (TC) formula used in realistic electronic structure calculations[8,9] and $\alpha_G^{(\mathrm{SF})}$ is the spin-flip (SF) formula used in certain toy-model calculations.[23] The discrepancy between TC and SF expressions stems from interband ($n \neq n'$) contributions to damping, which may now connect states with *different* band energies due to the disorder broadening of the spectral functions. Therefore, $\langle \vec{k}n|[\mathcal{H}_{\mathrm{KS}}, s_\alpha]|\vec{k}n'\rangle$ no longer vanishes for $n \neq n'$ and Eq. (27) indicates that $\alpha_G^{(\mathrm{TC})} \simeq \alpha_G^{(\mathrm{SF})}$ only if the Gilbert damping is dominated by intraband contributions and/or if the energy difference between the states connected by interband transitions is small compared to Δ. When $\alpha_G^{(\mathrm{TC})} \neq \alpha_G^{(\mathrm{SF})}$, it is *a priori* unclear which approach is the most accurate. One obvious flaw of the SF formula is that it produces a spurious damping in absence of spin-orbit interactions; this unphysical contribution originates from interband transitions and may be canceled out by adding the leading-order impurity vertex correction.[24] In contrast, $[\mathcal{H}_P, s_y]=0$ in absence of spin-orbit interaction and hence the TC formula vanishes identically, even without vertex corrections. From this analysis, TC appears to have a pragmatic edge over SF in materials with weak spin-orbit interaction. However, insofar as it allows interband transitions that connect states with $\omega_{i,j} > \Delta$, TC is not quantitatively reliable. Furthermore, it can be shown[22] that when the intrinsic spin-orbit coupling is significant (e.g., in ferromagnetic semiconductors), the advantage of TC over SF (or vice versa) is marginal and impurity vertex corrections play a significant role.

V. CONCLUSIONS

Using spin-density-functional theory we have derived a Stoner model expression for the Gilbert damping coefficient in itinerant ferromagnets. This expression accounts for atomic scale variations of the exchange self energy, as well as for arbitrary disorder and spin-orbit interaction. By treating disorder approximately, we have derived the spin-flip and torque-correlation formulas previously used in toy-model and *ab initio* calculations, respectively. We have traced the discrepancy between these equations to the treatment of interband transitions that connect states which are not close in energy. A better treatment of disorder, which requires the inclusion of impurity vertex corrections, will be the ultimate judge on the relative reliability of either approach. When damping is dominated by intraband transitions, a circumstance which we believe is common, the two formulas are identical and both are likely to provide reliable estimates.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation under Grant No. DMR-0547875.

[1] For a historical perspective, see T. L. Gilbert, IEEE Trans. Magn. **40**, 3443 (2004).
[2] For an introductory review, see D. C. Ralph and M. D. Stiles, J. Magn. Magn. Mater. **320**, 1190 (2008).
[3] *Ultrathin Magnetic Structures III: Fundamentals of Nanomagnetism*, edited by J. A. C. Bland and B. Heinrich (Springer-Verlag, New York, 2005).
[4] V. Korenman and R. E. Prange, Phys. Rev. B **6**, 2769 (1972).
[5] V. Kambersky, Czech. J. Phys., Sect. B **26**, 1366 (1976).
[6] Y. Tserkovnyak, G. A. Fiete, and B. I. Halperin, Appl. Phys. Lett. **84**, 5234 (2004); E. M. Hankiewicz, G. Vignale, and Y. Tserkovnyak, Phys. Rev. B **75**, 174434 (2007); Y. Tserkovnyak, H. J. Skadsem, A. Brataas, and G. E. W. Bauer, *ibid.* **74**, 144405 (2006); H. J. Skadsem, Y. Tserkovnyak, A. Brataas, and G. E. W. Bauer, *ibid.* **75**, 094416 (2007); H. Kohno, G. Tatara, and J. Shibata, J. Phys. Soc. Jpn. **75**, 113706 (2006); R. A. Duine, A. S. Nunez, J. Sinova, and A. H. MacDonald, Phys. Rev. B **75**, 214420 (2007); Y. Tserkovnyak, A. Brataas, and G. E. W. Bauer, J. Magn. Magn. Mater. **320**, 1282 (2008).
[7] D. Steiauf and M. Fahnle, Phys. Rev. B **72**, 064450 (2005); D. Steiauf, J. Seib, and M. Fahnle, *ibid.* **78**, 020410(R) (2008).
[8] K. Gilmore, Y. U. Idzerda, and M. D. Stiles, Phys. Rev. Lett. **99**, 027204 (2007).
[9] V. Kambersky, Phys. Rev. B **76**, 134416 (2007).
[10] O. Gunnarsson, J. Phys. F: Met. Phys. **6**, 587 (1976).
[11] Z. Qian and G. Vignale, Phys. Rev. Lett. **88**, 056404 (2002); K. Capelle and B. L. Gyorffy, Europhys. Lett. **61**, 354 (2003).
[12] Here we assume that the dependence of energy on magnetization direction which determines $\mathcal{H}_{\mathrm{eff}}$ is specified as a function of Ω_x and Ω_y only with Ω_z implicitly fixed by the constraint $\Omega_z=[1-\Omega_x^2-\Omega_y^2]^{1/2}$. If the free energy was expressed in a form with explicit Ω_z dependence we would find $\mathcal{H}_{\mathrm{eff},x}=-\partial F/\partial\Omega_x-(\partial F/\partial\Omega_z)(\partial\Omega_z/\partial\Omega_x)=-\partial F/\partial\Omega_x+(\partial F/\partial\Omega_z)\Omega_x$, where F is the free energy of the ferromagnet. Similarly we would find $\mathcal{H}_{\mathrm{eff},y}=-\partial F/\partial\Omega_y+(\partial F/\partial\Omega_z)\Omega_y$. The terms which arise from the Ω_z dependence of the free energy would more commonly be regarded as contributions to $\mathcal{H}_{\mathrm{eff},z}$. The difference is purely a matter of convention since both results would give the same value for $\hat{\Omega}\times\mathcal{H}_{\mathrm{eff}}$.
[13] In doing so we dodge the subtle difficulties which complicate theories of orbital magnetism in bulk metals. See, for example, J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett. **99**, 197202 (2007); I. Souza and D. Vanderbilt, Phys. Rev. B **77**, 054438 (2008) and work cited therein. This simplification should have little influence on the theory of damping because the orbital contribution to the magnetization is relatively small in systems of interest and because it in any event tends to be collinear with the spin magnetization.

[14] For most materials the FMR frequency is by far the smallest energy scale in the problem. Expansion to linear order is almost always appropriate.

[15] For zero-spin-orbit coupling α_G vanishes even in presence of magnetic impurities, provided that their spins follow the dynamics of the magnetization adiabatically.

[16] See, for example, A. C. Jenkins and W. M. Temmerman, Phys. Rev. B **60**, 10233 (1999) and work cited therein.

[17] While $\Delta(n,s) \sim n^{1/3}$ is no longer valid when correlation is included, even in this case Δ is inhomogeneous at the atomic length scale.

[18] This approximation does not preclude strong spatial variations of $|s_0(\vec{r})|$ and $|\Delta(\vec{r})|$ at atomic length scales; rather it is assumed that such spatial profiles will remain unchanged in the course of the magnetization dynamics.

[19] For notational simplicity we assume that all magnetic atoms are identical. Generalizations to magnetic compounds are straightforward.

[20] Equation (26) is valid provided that $\omega\tau \ll 1$, where τ is the quasiparticle lifetime. While this condition is normally satisfied in cases of practical interest, it invariably breaks down as $\tau \to \infty$. Hence the divergence of Eq. (26) in *perfect* crystals is spurious.

[21] In most systems of interest the main contribution to damping originates from a combination of intrinsic spin-orbit interactions and spin-independent disorder.

[22] I. Garate and A. H. MacDonald, Phys. Rev. B **79**, 064404 (2009)

[23] J. Sinova, T. Jungwirth, X. Liu, Y. Sasaki, J. K. Furdyna, W. A. Atkinson, and A. H. MacDonald, Phys. Rev. B **69**, 085209 (2004); In order to get the equivalence, trade h_z by Δ and use $\Delta = J_{pd} S_0$, where J_{pd} is the *p-d* exchange coupling between GaAs valence-band holes and Mn *d* orbitals. In addition, note that our spectral function differs from theirs by a factor 2π.

[24] H. Kohno, G. Tatara, and J. Shibata, J. Phys. Soc. Jpn. **75**, 113706 (2006).