Gilbert damping in conducting ferromagnets. II. Model tests of the torque-correlation formula

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We report on a study of Gilbert damping due to particle-hole pair excitations in conducting ferromagnets. We focus on a toy two-band model and on a four-band spherical model which provide an approximate description of ferromagnetic (Ga,Mn)As. These models are sufficiently simple that disorder-ladder-sum vertex corrections to the long-wavelength spin-spin response function can be summed to all orders. An important objective of this study is to assess the reliability of practical approximate expressions which can be combined with electronic structure calculations to estimate Gilbert damping in more complex systems.

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I. INTRODUCTION

The key role of the Gilbert parameter α_G in current-driven[1] and precessional[2] magnetization reversal has led to a renewed interest in this important magnetic material parameter. The theoretical foundations which relate Gilbert damping to the transverse spin-spin response function of the ferromagnet have been in place for some time.[3,4] It has nevertheless been difficult to predict trends as a function of temperature and across materials systems partly because damping depends on the strength and nature of the disorder in a manner that requires a more detailed characterization than is normally available. Two groups have recently[5] reported successful applications to transition-metal ferromagets of the *torque-correlation* formula[4–6] for α_G. This formula has the important advantage that its application requires knowledge only of the band structure, including its spin-orbit (SO) coupling, and of Bloch state lifetimes. The torque-correlation formula is physically transparent and can be applied with relative ease in combination with modern spin-density-functional-theory[7] (SDFT) electronic structure calculations. In this paper we compare the predictions of the torque-correlation formula with Kubo-formula self-consistent Born-approximation results for two different relatively simple model systems, an artificial two-band model of a ferromagnet with Rashba spin-orbit interactions, and a four-band model which captures the essential physics of (III,Mn)V ferromagnetic semiconductors.[8] The self-consistent Born-approximation theory for α_G requires that ladder-diagram vertex corrections be included in the transverse spin-spin response function. Since the Born approximation is exact[9] for weak scattering, we can use this comparison to assess the reliability of the simpler and more practical torque-correlation formula. We conclude that the torque-correlation formula is accurate when the Gilbert damping is dominated by intraband excitations of the transition-metal Fermi sea but that it can be inaccurate when it is dominated by interband excitations.

Our paper is organized as follows. In Sec. II we explain how we evaluate the transverse spin-spin response function for simple model ferromagnets. Section III discusses our result for the two-band Rashba model, while Sec. IV summarizes our findings for the four-band (III,Mn)V model. We conclude in Sec. V with a summary of our results and recommended *best practices* for the use of the torque-correlation formula.

II. GILBERT DAMPING AND TRANSVERSE SPIN-RESPONSE FUNCTION

A. Realistic SDFT versus *s-d* and *p-d* models

We view the two-band *s-d* and four-band *p-d* models studied in this paper as toy models which capture the essential features of metallic magnetism in systems that are, at least in principle,[10] more realistically described using SDFT. The *s-d* and *p-d* models correspond to the limit of *ab initio* SDFT in which (i) the majority-spin *d* bands are completely full and the minority-spin *d* bands are completely empty, (ii) hybridization between *s* or *p* and *d* bands is relatively weak, and (iii) there is exchange coupling between *d* and *s* or *p* moments. In a recent paper[6] we have proposed the following expression for the Gilbert-damping contribution from particle-hole excitations in SDFT bands:

$$\alpha_G = \frac{1}{S_0}\partial_\omega \,\mathrm{Im}[\tilde{\chi}^{\mathrm{QP}}_{x,x}], \tag{1}$$

where $\tilde{\chi}^{\mathrm{QP}}_{x,x}$ is a response function which describes how the quasiparticle bands change in response to a spatially smooth variation in magnetization orientation and S_0 is the total spin. Specifically,

$$\tilde{\chi}^{\mathrm{QP}}_{\alpha,\beta}(\omega) = \sum_{ij} \frac{f_j - f_i}{\omega_{ij} - \omega - i\eta} \langle j|s^\alpha \Delta_0(\vec{r})|i\rangle\langle i|s^\beta \Delta_0(\vec{r})|j\rangle, \tag{2}$$

where α and β label the x and y transverse spin directions and the easy direction for the magnetization is assumed to be the $\hat{z}$ direction. In Eq. (2) $|i\rangle$, f_i, and ω_{ij} are Kohn-Sham eigenspinors, Fermi factors, and eigenenergy differences, respectively, s_α is a spin operator, and $\Delta_0(\vec{r})$ is the difference between the majority-spin and minority-spin exchange-correlation potentials. In the *s-d* and *p-d* models $\Delta_0(\vec{r})$ is replaced by a phenomenological constant, which we denote by Δ_0 below. With $\Delta_0(\vec{r})$ replaced by a constant, $\tilde{\chi}^{\mathrm{QP}}_{x,x}$ reduces to a standard spin-response function for noninteracting quasiparticles in a possibly spin-dependent random static external potential. The evaluation of this quantity, and in

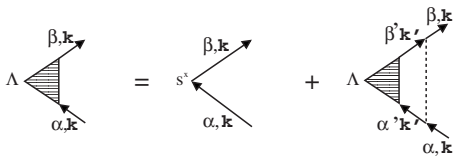

FIG. 1. Dyson equation for the renormalized vertex of the transverse spin-spin response function. The dotted line denotes impurity scattering.

particular the low-frequency limit in which we are interested, is nontrivial only because disorder plays an essential role.

B. Disorder perturbation theory

We start by writing the transverse spin-response function of a disordered metallic ferromagnet in the Matsubara formalism,

$$\tilde{\chi}_{xx}^{\mathrm{QP}}(i\omega) = -V\frac{\Delta_0^2}{\beta}\sum_{\omega_n} P(i\omega_n, i\omega_n + i\omega), \tag{3}$$

where the minus sign originates from fermionic statistics, V is the volume of the system, and

$$P(i\omega_n, i\omega_n + i\omega) \equiv \int \frac{d^D k}{(2\pi)^D}\Lambda_{\alpha,\beta}(i\omega_n, i\omega_n + i\omega; \mathbf{k}) G_\beta(i\omega_n + i\omega, \mathbf{k}) s^x_{\beta,\alpha}(\mathbf{k}) G_\alpha(i\omega_n, \mathbf{k}). \tag{4}$$

In Eq. (4) $|\alpha\mathbf{k}\rangle$ is a band eigenstate at momentum $\mathbf{k}$, D is the dimensionality of the system, $s^x_{\alpha,\beta}(\mathbf{k}) = \langle\alpha\mathbf{k}|s^x|\beta\mathbf{k}\rangle$ is the spin-flip matrix element, $\Lambda_{\alpha,\beta}(\mathbf{k})$ is its vertex-corrected counterpart (see below), and

$$G_\alpha(i\omega_n, \mathbf{k}) = \left[i\omega_n + E_F - E_{\mathbf{k},\alpha} + i\frac{1}{2\tau_{\mathbf{k},\alpha}}\mathrm{sgn}(\omega_n)\right]^{-1}. \tag{5}$$

We have included disorder within the Born approximation by incorporating a finite lifetime τ for the quasiparticles and by allowing for vertex corrections at one of the spin vertices.

The vertex function in Eq. (4) obeys the Dyson equation (Fig. 1),

$$\Lambda_{\alpha,\beta}(i\omega_n, i\omega_n + i\omega; \mathbf{k}) = s^x_{\alpha,\beta}(\mathbf{k}) + \int \frac{d^D k'}{(2\pi)^D} u^a(\mathbf{k} - \mathbf{k}') s^a_{\alpha,\alpha'}(\mathbf{k}, \mathbf{k}') G_{\alpha'}(i\omega_n, \mathbf{k}') \times \Lambda_{\alpha',\beta'}(i\omega_n, i\omega_n + i\omega; \mathbf{k}') G_{\beta'}(i\omega_n + i\omega, \mathbf{k}') \times s^a_{\beta',\beta}(\mathbf{k}', \mathbf{k}), \tag{6}$$

where $u^a(\mathbf{q}) \equiv n_a \overline{V_a^2}(\mathbf{q})$ $(a=0,x,y,z)$, n_a is the density of scatterers, $V_a(\mathbf{q})$ is the scattering potential [dimensions: (energy)$\times$(volume)], and the overline stands for disorder averaging.[11,12] Ward's identity requires that $u^a(\mathbf{q})$ and $\tau_{\mathbf{k},\alpha}$ be related via the Fermi golden rule,

$$\frac{1}{\tau_{\alpha\mathbf{k}}} = 2\pi\int_{\mathbf{k}'} u^a(\mathbf{k} - \mathbf{k}')\sum_{\alpha'} s^a_{\alpha,\alpha'} s^a_{\alpha',\alpha}\delta(E_{\mathbf{k}\alpha} - E_{\mathbf{k}'\alpha'}), \tag{7}$$

where $\int_{\mathbf{k}} \equiv \int d^D k/(2\pi)^D$. In this paper we restrict ourselves to spin-independent $(a=0)$ disorder and spin-dependent disorder oriented along the equilibrium-exchange-field direction $(a=z)$.[13] Performing the conventional[14] integration around the branch cuts of P, we obtain

$$\tilde{\chi}_{xx}^{\mathrm{QP}}(i\omega) = V\Delta_0^2\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi i} f(\epsilon)[P(\epsilon + i\delta, \epsilon + i\omega) - P(\epsilon - i\delta, \epsilon + i\omega) + P(\epsilon - i\omega, \epsilon + i\delta) - P(\epsilon - i\omega, \epsilon - i\delta)], \tag{8}$$

where $f(\epsilon)$ is the Fermi function. Next, we perform an analytical continuation $i\omega \to \omega + i\eta$ and take the imaginary part of the resulting retarded response function. Assuming low temperatures, this yields

$$\alpha_G = \frac{\Delta_0^2}{2\pi s_0}\{\mathrm{Re}[P(-i\delta, i\delta)] - \mathrm{Re}[P(i\delta, +i\delta)]\} = \frac{\Delta_0^2}{2\pi s_0}\mathrm{Re}(P^{A,R} - P^{R,R}), \tag{9}$$

where $s_0 = S_0/V$,

$$P^{R(A),R} = \int_{\mathbf{k}} \Lambda^{R(A),R}_{\alpha,\beta}(\mathbf{k}) G^R_\beta(0,\mathbf{k}) s^x_{\beta,\alpha}(\mathbf{k}) G^{R(A)}_\alpha(0,\mathbf{k}), \tag{10}$$

and $G^{R(A)}(0,\mathbf{k})$ is the retarded (advanced) Green's function at the Fermi energy. The principal difficulty of Eq. (9) resides in solving the Dyson equation for the vertex function. We first discuss our method of solution in general terms before turning in Secs. III and IV to its application to the *s-d* and *p-d* models.

C. Evaluation of impurity vertex corrections for multiband models

Equation (6) encodes disorder-induced diffusive correlations between itinerant carriers and is an integral equation of considerable complexity. Fortunately, it is possible to transform it into a relatively simple algebraic equation provided that the impurity potentials are short ranged in real space.

Referring back to Eq. (6) it is clear that the solution of the Dyson equation would be trivial if the vertex function was independent of momentum. That is certainly not the case in general because the matrix elements of the spin operators may be momentum dependent. Yet, for short-range scatterers the entire momentum dependence of the vertex matrix elements comes from the eigenstates alone,

$$s^a_{\alpha,\alpha'}(\mathbf{k}, \mathbf{k}') = \sum_{m,m'} \langle\alpha\mathbf{k}|m\rangle\langle m'|\alpha'\mathbf{k}'\rangle s^a_{m,m'}. \tag{11}$$

This property motivates our solution strategy which characterizes the momentum dependence of the vertex function by expanding it in terms of the eigenstates of s^z (s^x or s^y bases would work equally well),

$$\Lambda_{\alpha,\beta}(\mathbf{k}) = \langle\alpha\mathbf{k}|\Lambda|\beta\mathbf{k}\rangle = \sum_{m,m'}\langle\alpha\mathbf{k}|m\rangle\Lambda_{m,m'}\langle m'|\beta\mathbf{k}\rangle, \tag{12}$$

where $|m\rangle$ is an eigenstate of s^z, with eigenvalue m. Plugging Eqs. (11) and (12) into Eq. (6) demonstrates that, as expected, $\Lambda_{m,m'}$ is *independent* of momentum. After canceling

common factors from both sides of the resulting expression and using $\partial_{\mathbf{q}} u^a(\mathbf{q})=0$ $(a=0,z)$, we arrive at

$$\Lambda^{R(A),R}_{m,m'} = s^x_{m,m'} + \sum_{l,l'} U^{R(A),R}_{m,m':l,l'} \Lambda^{R(A),R}_{l,l'}, \tag{13}$$

where

$$U^{R(A),R}_{m,m':l,l'} \equiv (u^0 + u^z mm') \int_{\mathbf{k}} \langle m|\alpha\mathbf{k}\rangle G^{R(A)}_{\alpha}(0,\mathbf{k}) \langle \alpha\mathbf{k}|l\rangle \times \langle l'|\beta\mathbf{k}\rangle G^{R}_{\beta}(0,\mathbf{k}) \langle \beta\mathbf{k}|m'\rangle. \tag{14}$$

Equations (12)–(14) provide a solution for the vertex function that is significantly easier to analyze than the original Dyson equation.

III. GILBERT DAMPING FOR A MAGNETIC TWO-DIMENSIONAL ELECTRON GAS

The first model we consider is a two-dimensional electron-gas (2DEG) model with ferromagnetism and Rashba spin-orbit interactions. We refer to this as the magnetic 2DEG (M2DEG) model. This toy model is almost never even approximately realistic,[15] but a theoretical study of its properties will prove useful in a number of ways. First, it is conducive to a fully analytical evaluation of the Gilbert damping, which will allow us to precisely understand the role of different actors. Second, it enables us to explain in simple terms why higher-order vertex corrections are significant when there is spin-orbit interaction in the band structure. Third, as we demonstrate below the Gilbert damping of a M2DEG has qualitative features similar to those of (Ga,Mn)As.

The band Hamiltonian of the M2DEG model is

$$H = \frac{k^2}{2m} + \mathbf{b}_{\mathbf{k}} \cdot \sigma, \tag{15}$$

where $\mathbf{b}_{\mathbf{k}}=(-\lambda k_y, \lambda k_x, \Delta_0)$, Δ_0 is the difference between majority- and minority-spin exchange-correlation potentials, λ is the strength of the Rashba SO coupling, and $\vec{\sigma}=2\vec{s}$ is a vector of Pauli matrices. The corresponding eigenvalues and eigenstates are

$$E_{\pm,\mathbf{k}} = \frac{k^2}{2m} \pm \sqrt{\Delta_0^2 + \lambda^2 k^2}, \tag{16}$$

$$|\alpha\mathbf{k}\rangle = e^{-is^z\phi} e^{-is^y\theta} |\alpha\rangle, \tag{17}$$

where $\phi=-\tan^{-1}(k_x/k_y)$ and $\theta=\cos^{-1}(\Delta_0/\sqrt{\Delta_0^2+\lambda^2k^2})$ are the spinor angles and $\alpha=\pm$ is the band index. It follows that

$$\langle m|\alpha,\mathbf{k}\rangle = \langle m|e^{-is^z\phi} e^{-is^y\theta}|\alpha\rangle = e^{-im\phi} d_{m,\alpha}(\theta), \tag{18}$$

where $d_{m,\alpha}=\langle m|e^{-is^y\theta}|\alpha\rangle$ is a Wigner function for $J=1/2$ angular momentum.[16] With these simple spinors, the azimuthal integral in Eq. (14) can be performed analytically to obtain

$$U^{R(A),R}_{m,m':l,l'} = \delta_{m-m',l-l'}(u^0 + u^z mm') \sum_{\alpha,\beta} \int \frac{dkk}{2\pi} d_{m\alpha} G^{R(A)}_{\alpha} \times (k) d_{l\alpha}(\theta) d_{m'\beta}(\theta) G^{R}_{\beta}(k) d_{l'\beta}(\theta), \tag{19}$$

where the Kronecker delta reflects the conservation of the angular momentum along z, owing to the azimuthal symmetry of the problem. In Eq. (19)

$$d_{m,m'} = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}, \tag{20}$$

and the retarded and advanced Green's functions are

$$G^{R(A)}_{+} = \frac{1}{-\xi_k - b_k + (-)i\gamma_+},$$

$$G^{R(A)}_{-} = \frac{1}{-\xi_k + b_k + (-)i\gamma_-}, \tag{21}$$

where $\xi_k=\frac{k^2-k_F^2}{2m}$, $b_k=\sqrt{\Delta_0^2+\lambda^2k^2}$, and $\gamma_\pm$ is (half) the golden-rule scattering rate of the band quasiparticles. In addition, Eq. (13) is readily inverted to yield

$$\Lambda^{R(A),R}_{+,+} = \Lambda^{R(A),R}_{-,-} = 0,$$

$$\Lambda^{R(A),R}_{+,-} = \frac{1}{2} \frac{1}{1 - U^{R(A),R}_{+,-:+,-}},$$

$$\Lambda^{R(A),R}_{-,+} = \frac{1}{2} \frac{1}{1 - U^{R(A),R}_{-,+:-,+}}. \tag{22}$$

In order to make further progress analytically we assume that $(\Delta_0, \lambda k_F, \gamma) \ll E_F = k_F^2/2m$. It then follows that $\gamma_+ \simeq \gamma_- \equiv \gamma$ and that $\gamma = \pi N_{2D} u^0 + \pi N_{2D} \frac{u^z}{4} \equiv \gamma_0 + \gamma_z$. Equations (19) and (20) combine to give

$$U^{R,R}_{-,+:-,+} = U^{R,R}_{+,-:+,-} = 0,$$

$$U^{A,R}_{-,+:-,+} = (\gamma_0 - \gamma_z) \left[\frac{i}{-b + i\gamma} \cos^4\left(\frac{\theta}{2}\right) + \frac{i}{b + i\gamma} \sin^4\left(\frac{\theta}{2}\right) + \frac{2}{\gamma} \cos^2\left(\frac{\theta}{2}\right) \sin^2\left(\frac{\theta}{2}\right) \right],$$

$$U^{A,R}_{+,-:+,-} = (U^{A,R}_{-,+:-,+})^\star, \tag{23}$$

where $b \simeq \sqrt{\lambda^2 k_F^2 + \Delta_0^2}$ and $\cos\theta \simeq \Delta_0/b$. The first and second terms in square brackets in Eq. (23) emerge from interband transitions [$\alpha \neq \beta$ in Eq. (19)], while the last term stems from intraband transitions ($\alpha=\beta$). Amusingly, U vanishes when the spin-dependent scattering rate equals the Coulomb scattering rate ($\gamma_z=\gamma_0$); in this particular instance vertex corrections are completely absent. On the other hand, when $\gamma_z=0$ and $b \ll \gamma$ we have $U^{A,R}_{-,+:-,+} \simeq U^{A,R}_{+,-:+,-} \simeq 1$, implying that vertex corrections strongly enhance Gilbert damping [recall Eq. (22)]. We will discuss the role of vertex corrections more fully below.

After evaluating $\Lambda(\mathbf{k})$ from Eqs. (12), (22), and (23), the last step is to compute

$$P^{R(A),R} = \int_{\mathbf{k}} \Lambda^{R(A),R}_{\alpha,\beta}(\mathbf{k}) s^{x}_{\beta,\alpha}(\mathbf{k}) G^{R(A)}_{\alpha}(\mathbf{k}) G^{R}_{\beta}(\mathbf{k}). \quad (24)$$

Since we are assuming that the Fermi energy is the largest energy scale, the integrand in Eq. (24) is sharply peaked at the Fermi surface, leading to $P^{R,R} \simeq 0$. In the case of spin-independent scatterers ($\gamma_z = 0 \to \gamma = \gamma_0$), tedious but straightforward algebra takes us to

$$\alpha_G(u^z = 0) = \frac{N_{2D}\Delta_0^2}{4 s_0 \gamma_0} \frac{(\lambda^2 k_F^2)(b^2 + \Delta_0^2 + 2\gamma_0^2)}{(b^2 + \Delta_0^2)^2 + 4\Delta_0^2 \gamma_0^2}. \quad (25)$$

Equation (29) agrees with the results published in the recent literature.[17] We note that $\alpha_G(u^z=0)$ vanishes in the absence of SO interactions, as expected. It is illustrative to expand Eq. (25) in the $b \gg \gamma_0$ regime,

$$\alpha_G(u^z = 0) \simeq \frac{N_{2D}\Delta_0^2}{2 s_0} \left[\frac{\lambda^2 k_F^2}{2(b^2 + \Delta_0^2)} \frac{1}{\gamma_0} + \frac{\lambda^4 k_F^4}{(b^2 + \Delta_0^2)^3} \gamma_0 \right], \quad (26)$$

which displays intraband ($\sim \gamma_0^{-1}$) and interband ($\sim \gamma_0$) contributions separately. The intraband damping is due to the dependence of band eigenenergies on magnetization orientation—the *breathing Fermi-surface* effect[4] which produces more damping when the band quasiparticles scatter infrequently because the population distribution moves further from equilibrium. The intraband contribution to damping therefore tends to scale with the conductivity. For stronger disorder, the interband term in which scattering relaxes spin orientations takes over and α_G is proportional to the resistivity. Insofar as phonon scattering can be treated as elastic, the Gilbert damping will often show a nonmonotonic temperature dependence with the intraband mechanism dominating at low temperatures when the conductivity is large and the interband mechanism dominating at high temperatures when the resistivity is large.

For completeness, we also present analytic results for the case where $\gamma = \gamma_z$ in the $b \gg \gamma_z$ regime,

$$\alpha_G(u^0 = 0) \simeq \frac{N_{2D}\Delta_0^2}{2 s_0} \left[\frac{1}{\gamma_z} \frac{\lambda^2 k_F^2}{6b^2 - 2\Delta_0^2} + \gamma_z \frac{3b^4 + 6b^2\Delta_0^2 - \Delta_0^4}{(3b^2 - \Delta_0^2)^3} \right]. \quad (27)$$

This expression illustrates that SO interactions in the band structure are a necessary condition for the intraband transition contribution to α_G. The interband contribution survives in the absence of SO as long as the disorder potential is spin dependent. Interband scattering is possible for spin-dependent disorder because majority and minority-spin states on the Fermi surface are not orthogonal when their potentials are not identical. Note incidentally the contrast between Eqs. (26) and (27)—in the former the interband coefficient is most suppressed at weak intrinsic SO interaction while in the latter it is the intraband coefficient which gets weakest for small λk_F.

More general cases relaxing the $(\Delta_0, \lambda k_F, \gamma) \ll E_F$ assumption must be studied numerically; the results are collected in Figs. 2–4. Figure 2 highlights the inadequacy of completely neglecting vertex corrections in the limit of weak spin-orbit interaction; the inclusion of the leading-order vertex correction largely solves the problem. However, Figs. 2 and 3 together indicate that higher-order vertex corrections are noticeable when disorder or spin-orbit coupling is strong. In light of the preceding discussion the monotonic decay in Fig.

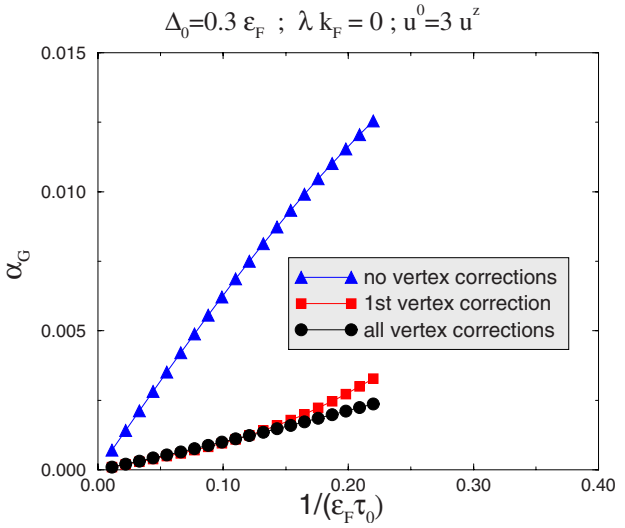

FIG. 2. (Color online) M2DEG: Gilbert damping in the absence of spin-orbit coupling. When the intrinsic spin-orbit interaction is small, the first vertex correction is sufficient for the evaluation of Gilbert damping provided that the ferromagnet exchange splitting is large compared to the lifetime broadening of the quasiparticle energies. For more disordered ferromagnets ($E_F\tau_0 < 5$ in this figure) higher-order vertex corrections begin to matter. In either case vertex corrections are significant. In this figure $1/\tau_0$ stands for the scattering rate off spin-independent impurities, defined as a two-band average at the Fermi energy, and the spin-dependent and spin-independent impurity strengths are chosen to satisfy $u^0 = 3u^z$.

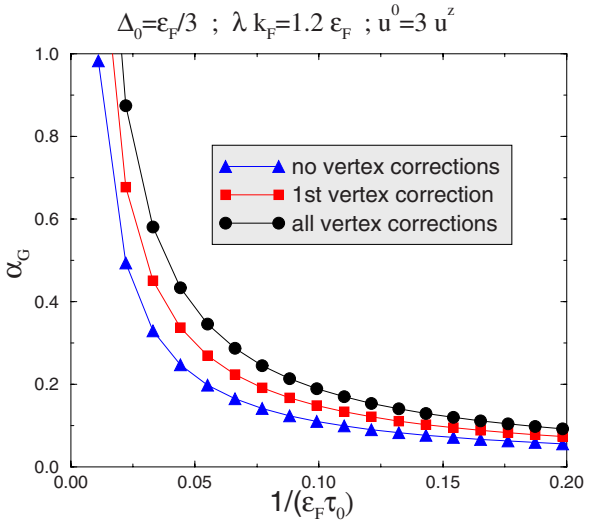

FIG. 3. (Color online) M2DEG: Gilbert damping for strong SO interactions ($\lambda k_F = 1.2 E_F \simeq 4\Delta_0$). In this case higher-order vertex corrections matter (up to 20%) even at low disorder. This suggests that higher-order vertex corrections will be important in real ferromagnetic semiconductors because their intrinsic SO interactions are generally stronger than their exchange splittings.

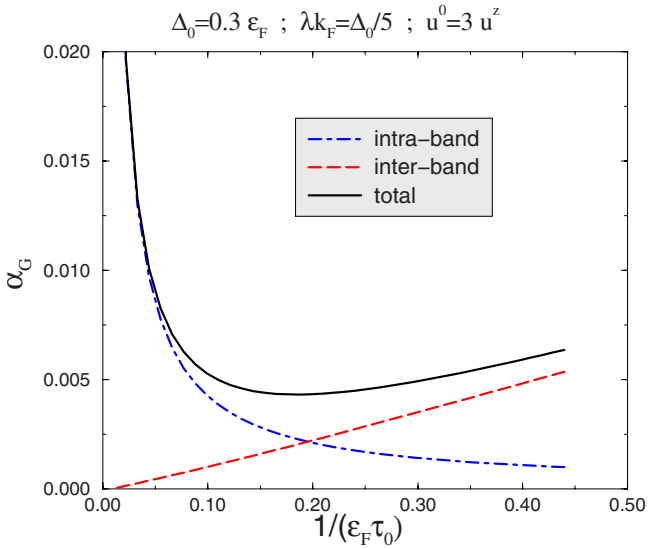

FIG. 4. (Color online) M2DEG: Gilbert damping for moderate SO interactions ($\lambda k_F=0.2\Delta_0$). In this case there is a crossover between the intraband dominated and the interband dominated regimes, which gives rise to a nonmonotonic dependence of Gilbert damping on disorder strength. The stronger the intrinsic SO relative to the exchange field is, the higher is the value of disorder at which the crossover occurs. This is why the damping is monotonically increasing with disorder in Fig. 2 and monotonically decreasing in Fig. 3.

3 may appear surprising because the interband contribution presumably increases with γ. Yet, this argument is strictly correct only for weakly spin-orbit coupled systems, where the crossover between interband and intraband dominated regimes occurs at low disorder. For strongly spin-orbit coupled systems the crossover may take place at a scattering rate that is (i) beyond experimental relevance and/or (ii) larger than the band splitting, in which case the interband contribution behaves much like its intraband partner, i.e., $O(1/\gamma)$. Nonmonotonic behavior is restored when the spin-orbit splitting is weaker, as shown in Fig. 4.

Finally, our analysis opens an opportunity to quantify the importance of higher-order impurity vertex corrections. Kohno *et al.*[12] claimed that the bare vertex along with the *first* vertex correction fully captures the Gilbert damping of a ferromagnet provided that $\Delta_0\tau \gg 1$. To first order in U the vertex function is

$$\Lambda^{R(A),R}_{m,m'} = s^x_{m,m'} + \sum_{ll'} U^{R(A),R}_{m,m';l,l'} s^x_{l,l'}. \tag{28}$$

Taking $\gamma=\gamma_z$ for simplicity, we indeed get

$$\lim_{\lambda\to 0} \alpha_G \simeq A\gamma + O(\gamma^2),$$

$$\frac{A(1)}{A(\infty)} = 1, \tag{29}$$

where $A(1)$ contains the first vertex correction only and $A(\infty)$ includes all vertex corrections. However, the state of affairs changes after turning on the intrinsic SO interaction, whereupon Eq. (29) transforms into

$$\alpha_G(\lambda \neq 0) \simeq B\gamma + C\frac{1}{\gamma},$$

$$\frac{B(1)}{B(\infty)} = \frac{\Delta_0^2(3b^2-\Delta_0^2)^3(3b^2+\Delta_0^2)}{4b^6(3b^4+6b^2\Delta_0^2-\Delta_0^4)},$$

$$\frac{C(1)}{C(\infty)} = \frac{(b^2+\Delta_0^2)(3b^2-\Delta_0^2)}{4b^4}. \tag{30}$$

When $\Delta_0 \ll \lambda k_F$, *both* intraband and interband ratios show a significant deviation from unity,[18] to which they converge as $\lambda \to 0$. In order to understand this behavior, let us look back at Eq. (22). There, we can formally expand the vertex function as $\Lambda = \frac{1}{2}\Sigma_{n=0}^{\infty} U^n$, where the nth-order term stems from the nth vertex correction. From Eq. (23) we find that when $\lambda = 0$, $U^n \sim O(\gamma^n)$ and thus $n \geq 2$ vertex corrections will not matter for the Gilbert damping, which is $O(\gamma)$ (Ref. 19) when $E_F \gg \gamma$. In contrast, when $\lambda \neq 0$ the intraband term in Eq. (23) is no longer zero, and consequently *all* powers of U contain $O(\gamma^0)$ and $O(\gamma^1)$ terms. In other words, all vertices contribute to $O(1/\gamma)$ and $O(\gamma)$ in the Gilbert damping, especially if $\lambda k_F/\Delta_0$ is not small. This conclusion should prove valid beyond the realm of the M2DEG because it relies only on the mantra "intraband $\sim O(1/\gamma)$, interband $\sim O(\gamma)$." Our expectation that higher-order vertex corrections be important in (Ga,Mn)As will be confirmed numerically in Sec. IV.

IV. GILBERT DAMPING FOR (Ga,Mn)As

(Ga,Mn)As and other (III,Mn)V ferromagnets are like transition metals in that their magnetism is carried mainly by d orbitals but are unlike transition metals in that neither majority nor minority-spin d orbitals are present at the Fermi energy. The orbitals at the Fermi energy are very similar to the states near the top of the valence band of the host (III,V) semiconductor, although they are of course weakly hybridized with the minority- and majority-spin d orbitals. For this reason the electronic structure of (III,Mn)V ferromagnets is extremely simple and can be described reasonably accurately with the phenomenological model which we employ in this section. Because the top of the valence band in (III,V) semiconductors is split by spin-orbit interactions, spin-orbit coupling plays a dominant role in the bands of these ferromagnets. An important consequence of the strong SO interaction in the band structure is that diffusive vertex corrections influence α_G significantly at all orders; this is the central idea of this section.

Using a p-d mean-field theory model[8] for the ferromagnetic ground state and a four-band spherical model[20] for the host semiconductor band structure, $Ga_{1-x}Mn_xAs$ may be described by

$$H = \frac{1}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_3(\mathbf{k}\cdot\mathbf{s})^2\right] + \Delta_0 s^z, \tag{31}$$

where $\mathbf{s}$ is the spin operator projected onto the $J=3/2$ total angular-momentum subspace at the top of the valence band

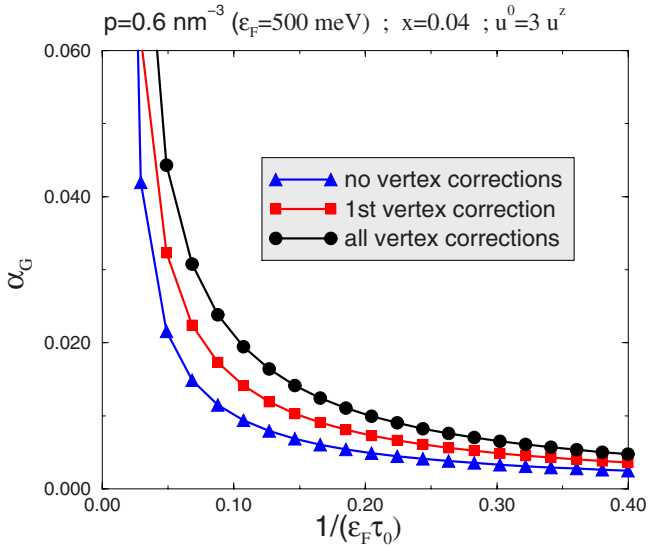

FIG. 5. (Color online) GaMnAs: higher-order vertex corrections make a significant contribution to Gilbert damping due to the prominent spin-orbit interaction in the band structure of GaAs. x is the Mn fraction, and p is the hole concentration that determines the Fermi energy E_F. In this figure, the spin-independent impurity strength u^0 was taken to be three times larger than the magnetic impurity strength u^z. $1/\tau_0$ corresponds to the scattering rate off Coulomb impurities and is evaluated as a four-band average at the Fermi energy.

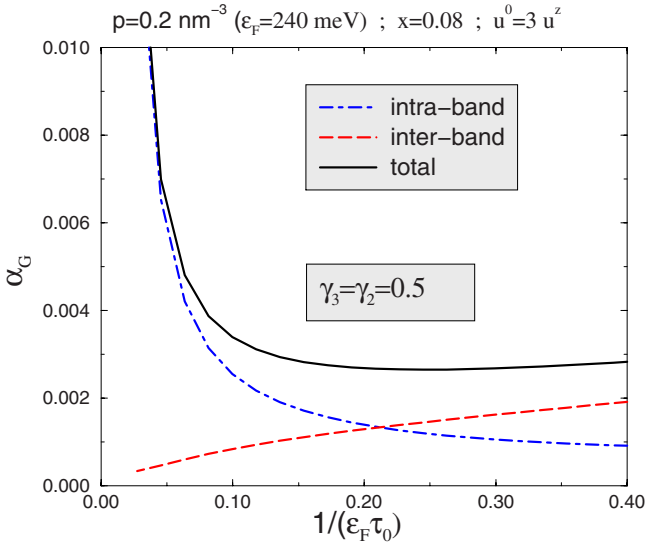

FIG. 6. (Color online) GaMnAs: when the spin-orbit splitting is reduced (in this case by reducing the hole density to 0.2 nm^{-3} and artificially taking γ_3=0.5), the crossover between interband and intraband dominated regimes produces a nonmonotonic shape of the Gilbert damping, much like in Fig. 4. When either γ_2 or p is made larger or x is reduced, we recover the monotonic decay of Fig. 5.

and $\{\gamma_1=6.98,\ \gamma_2=\gamma_3=2.5\}$ are the Luttinger parameters for the spherical-band approximation to GaAs. In addition, $\Delta_0=J_{p\text{-}d}SN_{\mathrm{Mn}}$ is the exchange field, $J_{p\text{-}d}=55$ meV nm^3 is the p-d exchange coupling, $S=5/2$ is the spin of the Mn ions, $N_{\mathrm{Mn}}=4x/a^3$ is the density of Mn ions, and $a=0.565$ nm is the lattice constant of GaAs.

The $\Delta_0=0$ eigenstates of this model are

$$|\tilde{\alpha},\mathbf{k}\rangle = e^{-is^z\phi}e^{-is^y\theta}|\tilde{\alpha}\rangle, \tag{32}$$

where $|\tilde{\alpha}\rangle$ is an eigenstate of s^z with eigenvalue $\tilde{\alpha}$. Unfortunately, the analytical form of the $\Delta_0\neq 0$ eigenstates is unknown. Nevertheless, since the exchange field preserves the azimuthal symmetry of the problem, the ϕ dependence of the full eigenstates $|\alpha\mathbf{k}\rangle$ will be identical to that of Eq. (32). This observation leads to $U_{m,m';l,l'}\propto\delta_{m-m',l-l'}$, which simplifies Eq. (14). α_G can be calculated numerically following the steps detailed in Secs. I and II; the results are summarized in Figs. 5 and 6. Note that vertex corrections moderately increase the damping rate, as in the case of a M2DEG model with strong spin-orbit interactions. Figure 5 underlines both the importance of higher-order vertex corrections in (Ga,Mn)As and the monotonic decay of the damping as a function of scattering rate. The latter signals the supremacy of the intraband contribution to damping, accentuated at larger hole concentrations. Had the intrinsic spin-orbit interaction been substantially weaker,[21] α_G would have traced a nonmonotonic curve as shown in Fig. 6. The degree to which the intraband breathing Fermi-surface model effect dominates depends on the details of the band structure and can be influenced by corrections to the spherical model which we have adopted here to simplify the vertex-correction calculation. The close correspondence between Figs. 5 and 6 and Figs. 3 and 4 reveals the success of the M2DEG as a versatile gateway for realistic models and justifies the extensive attention devoted to it in this paper and elsewhere.

V. ASSESSMENT OF THE TORQUE-CORRELATION FORMULA

Thus far we have evaluated the Gilbert damping for a M2DEG model and a (Ga,Mn)As model using the (bare) spin-flip vertex $\langle\alpha,\mathbf{k}|s^x|\beta,\mathbf{k}\rangle$ and its renormalized counterpart $\langle\alpha,\mathbf{k}|\Lambda|\beta,\mathbf{k}\rangle$. The vertex-corrected results are expected to be exact for $1/\tau$ small compared to the Fermi energy. For practical reasons, state-of-the-art band-structure calculations[5] forgo impurity vertex corrections altogether and instead employ the torque-correlation matrix element, which we shall denote as $\langle\alpha,\mathbf{k}|K|\beta,\mathbf{k}\rangle$ (see below for an explicit expression). In this section we compare damping rates calculated using $s^x_{\alpha,\beta}$ vertices with those calculated using $K_{\alpha,\beta}$ vertices. We also compare both results with the exact damping rates obtained by using $\Lambda_{\alpha,\beta}$. The ensuing discussion overlaps with and extends our recent preprint.[6]

We shall begin by introducing the following identity:[4]

$$\begin{aligned}\langle\alpha,\mathbf{k}|s^x|\beta,\mathbf{k}\rangle &= i\langle\alpha,\mathbf{k}|[s^z,s^y]|\beta,\mathbf{k}\rangle \\ &= \frac{i}{\Delta_0}(E_{\mathbf{k},\alpha}-E_{\mathbf{k},\beta})\langle\alpha,\mathbf{k}|s^y|\beta,\mathbf{k}\rangle \\ &\quad -\frac{i}{\Delta_0}\langle\alpha,\mathbf{k}|[H_{\mathrm{so}},s^y]|\beta,\mathbf{k}\rangle.\end{aligned} \tag{33}$$

In Eq. (33) we have decomposed the mean-field quasiparticle Hamiltonian into a sum of spin-independent, exchange spin-

splitting, and other spin-dependent terms $H=H_{\rm kin}+H_{\rm so}+H_{\rm ex}$, where $H_{\rm kin}$ is the kinetic (spin-independent) part, $H_{\rm ex}=\Delta_0 s^z$ is the exchange spin-splitting term, and $H_{\rm so}$ is the piece that contains the intrinsic spin-orbit interaction. The last term on the right-hand side of Eq. (33) is the torque-correlation matrix element used in band-structure computations,

$$\langle \alpha,\mathbf{k}|K|\beta,\mathbf{k}\rangle \equiv -\frac{i}{\Delta_0}\langle \alpha,\mathbf{k}|[H_{\rm so},s^y]|\beta,\mathbf{k}\rangle. \tag{34}$$

Equation (33) allows us to make a few general remarks on the relation between the spin-flip and torque-correlation matrix elements. For intraband matrix elements, one immediately finds that $s^x_{\alpha,\alpha}=K_{\alpha,\alpha}$ and hence the two approaches agree. For interband matrix elements the agreement between $s^x_{\alpha,\beta}$ and $K_{\alpha,\beta}$ should be nearly identical when the first term in the final form of Eq. (33) is small, i.e., when[22] $(E_{\mathbf{k},\alpha}-E_{\mathbf{k},\beta}) \ll \Delta_0$. Since this requirement cannot be satisfied in the M2DEG, we expect that the interband contributions from K and s^x will always differ significantly in this model. More typical models, such as the four-band model for (Ga,Mn)As, have band crossings at a discrete set of k points, in the neighborhood of which $K_{\alpha,\beta}\simeq s^x_{\alpha,\beta}$. The relative weight of these crossing points in the overall Gilbert damping depends on a variety of factors. First, in order to make an impact they must be located within a shell of thickness $1/\tau$ around the Fermi surface. Second, the contribution to damping from those special points must outweigh that from the remaining k points in the shell; this might be the case for instance in materials with weak spin-orbit interaction and weak disorder, where the contribution from the crossing points would go like τ (large) while the contribution from points far from the crossings would be $\sim 1/\tau$ (small). Only if these two conditions are fulfilled should one expect good agreement between the interband contributions from spin-flip and torque-correlation formulas. When vertex corrections are included, of course, the same result should be obtained using either form for the matrix element since all matrix elements are between essentially degenerate electronic states when disorder is treated nonperturbatively.[6,17]

In the remaining part of this section we shall focus on a more quantitative comparison between the different formulas. For the M2DEG it is straightforward to evaluate α_G analytically using K instead of s^x and neglecting vertex corrections; we obtain

$$\alpha_G^K=\frac{N_{2D}\Delta_0}{8s_0}\left[\frac{\lambda^2k_F^2}{b^2}\frac{\Delta_0}{\gamma}+\left(\frac{\lambda^2k_F^2}{\Delta_0 b}\right)^2\frac{\gamma\Delta_0}{\gamma^2+b^2}\right], \tag{35}$$

where we assumed $(\gamma,\lambda k_F,\Delta_0)\ll\epsilon_F$. By comparing Eq. (35) with the exact expression Eq. (25), we find that the intraband parts are in excellent agreement when $\Delta_0\ll\lambda k_F$, i.e., when vertex corrections are relatively unimportant. In contrast, the interband parts differ markedly regardless of the vertex corrections. These trends are captured by Figs. 7 and 8, which compare the Gilbert damping obtained from s^x, K, and Λ matrix elements. Figure 7 corresponds to the weak spin-orbit limit, where it is found that in disordered ferromagnets s^x may grossly overestimate the Gilbert damping because its interband contribution does not vanish even as SO tends to zero. As explained in Sec. III, this flaw may be repaired by adding the leading-order impurity vertex correction. The torque-correlation formula is free from such problem because K vanishes identically in absence of SO interaction. Thus the main practical advantage of K is that it yields a physically sensible result without having to resort to vertex corrections. Continuing with Fig. 7, at weak disorder the intraband contributions dominate and therefore s^x and K coincide; even Λ agrees because for intraband transitions at

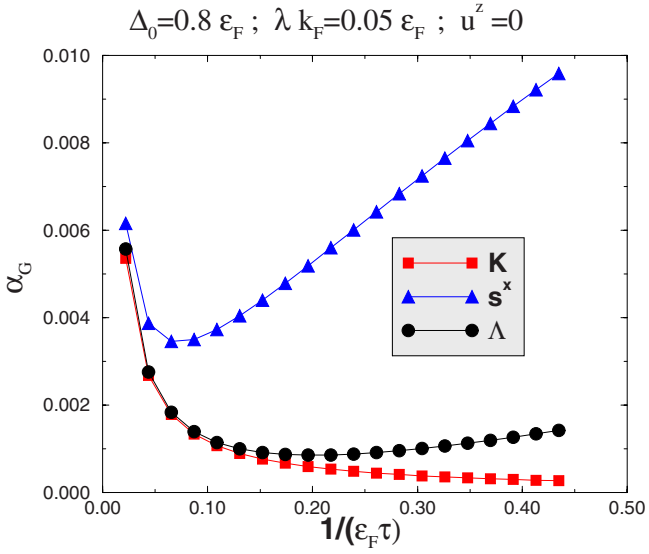

FIG. 7. (Color online) M2DEG: comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex-corrected result. In this figure the intrinsic spin-orbit interaction is relatively weak ($\lambda k_F=0.05E_F\simeq 0.06\Delta_0$) and we have taken $u^z=0$. The torque-correlation formula does not distinguish between spin-dependent and spin-independent disorders.

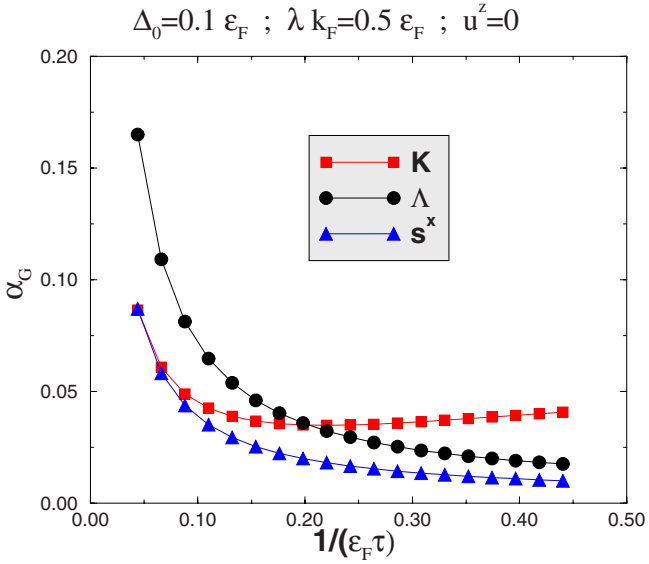

FIG. 8. (Color online) M2DEG: comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex-corrected result. In this figure the intrinsic spin-orbit interaction is relatively strong ($\lambda k_F=0.5E_F=5\Delta_0$) and we have taken $u^z=0$.

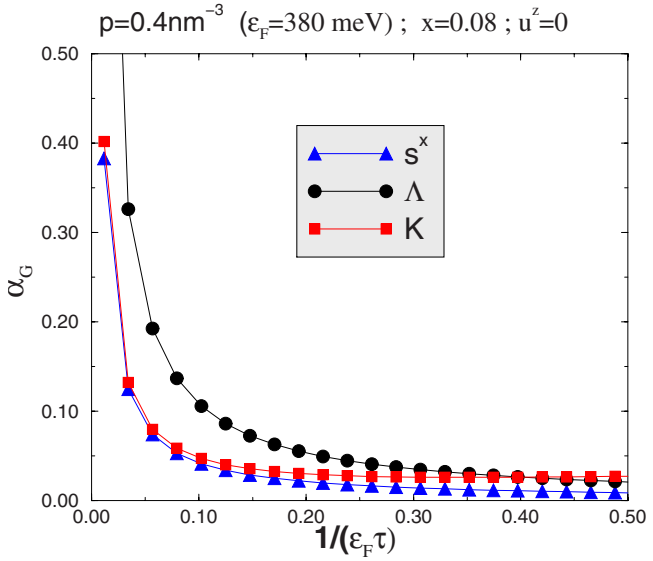

FIG. 9. (Color online) GaMnAs: comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex-corrected result. p is the hole concentration that determines the Fermi energy E_F and x is the Mn fraction. Due to the strong intrinsic SO, this figure shows similar features as those of Fig. 8.

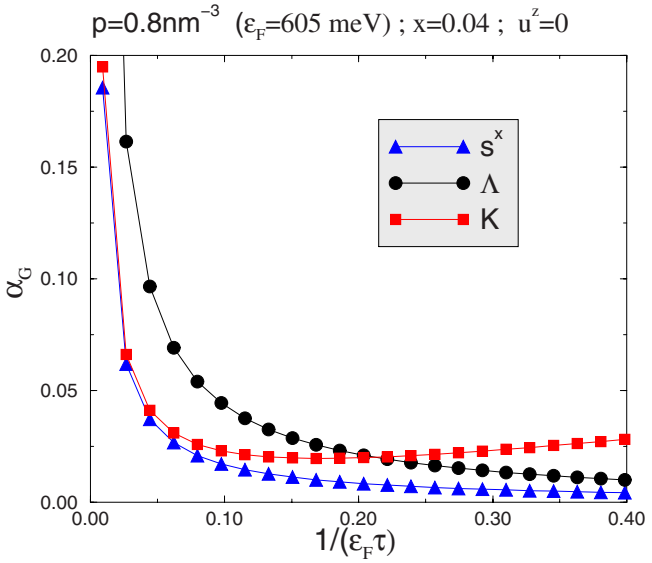

FIG. 10. (Color online) GaMnAs: comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex-corrected result. In relation to Fig. 9 the effective spin-orbit interaction is stronger due to a larger p and a smaller x.

weak spin-orbit interaction the vertex corrections are unimportant. Figure 8 corresponds to the strong spin-orbit case. In this case, at low disorder s^x and K agree well with each other but differ from the exact result because higher-order vertex corrections alter the intraband part substantially. For a similar reason, neither s^x nor K agrees with the exact Λ at higher disorder. Based on these model calculations, we do not believe that there are any objective grounds to prefer either the K torque-correlation or the s^x spin-flip formula estimate of α_G when spin-orbit interactions are strong and α_G is dominated by interband relaxation. A precise estimation of α_G under these circumstances appears to require that the character of disorder, including its spin dependence, be accounted for reliably and that the vertex-correction Dyson equation be accurately solved. Carrying out this program remains a challenge both because of technical complications in performing the calculation for general band structures and because disorder may not be sufficiently well characterized.

Analogous considerations apply for Figs. 9 and 10, which show results for the four-band model related to (Ga,Mn)As. These figures show results similar to those obtained in the strong spin-orbit limit of the M2DEG (Fig. 8). Overall, our study indicates that the torque-correlation formula captures the intraband contributions accurately when the vertex corrections are unimportant, while it is less reliable for interband contributions unless the predominant interband transitions connect states that are close in energy. The torque-correlation formula has the practical advantage that it correctly gives a zero-spin relaxation rate when there is no spin-orbit coupling in the band structure and spin-independent disorder. The damping it captures derives entirely from spin-orbit coupling in the bands. It therefore incorrectly predicts, for example, that the damping rate vanishes when spin-orbit coupling is absent in the bands and the disorder potential is spin dependent. Nevertheless, assuming that the dominant disorder is normally spin independent, the K formula may have a pragmatic edge over the s^x formula in weakly spin-orbit coupled systems. In strongly spin-orbit coupled systems there appears to be little advantage of one formula over the other. We recommend that interband and intraband contributions be evaluated separately when α_G is evaluated using the torque-correlation formula. For the intraband contribution the s^x and K lifetime formulas are identical. The model calculations reported here suggest that vertex corrections to the intraband contribution do not normally have an overwhelming importance. We conclude that α_G can be evaluated relatively reliably when the intraband contribution dominates. When the interband contribution dominates it is important to assess whether or not the dominant contributions are coming from bands that are nearby in momentum space, or equivalently whether or not the matrix elements which contribute originate from pairs of bands that are energetically spaced by much less than the exchange spin splitting at the same wave vector. If the dominant contributions are from nearby bands, the damping estimate should have the same reliability as the intraband contribution. If not, we conclude that the α_G estimate should be regarded with caution.

To summarize, this paper describes an evaluation of Gilbert damping for two simple models: a two-dimensional electron-gas ferromagnet model with Rashba spin-orbit interactions and a four-band model which provides an approximate description of (III, Mn)V of ferromagnetic semiconductors. Our results are exact in the sense that they combine time-dependent mean-field theory[6] with an impurity ladder sum to all orders, hence giving us leverage to make the following statements. First, previously neglected higher-order vertex corrections become quantitatively significant when the intrinsic spin-orbit interaction is larger than the exchange

splitting. Second, strong intrinsic spin-orbit interaction leads to the supremacy of intraband contributions in (Ga,Mn)As, with the corresponding monotonic decay of the Gilbert damping as a function of disorder. Third, the spin-torque formalism used in *ab initio* calculations of the Gilbert damping is quantitatively reliable as long as the intraband contributions dominate *and* the exchange field is weaker than the spin-orbit splitting; if these conditions are not met, the use of the spin-torque matrix element in a lifetime approximation formula offers no significant improvement over the original spin-flip matrix element.

ACKNOWLEDGMENTS

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[9] The Born approximation is no longer accurate at high impurity concentrations in which electron localization plays a role; however, localization effects are weak in transition-metal ferromagnets and metallic (Ga,Mn)As.

[10] These simplified models sometimes have the advantage that their parameters can be adjusted phenomenologically to fit experiments, compensating for inevitable inaccuracies in *ab initio* electronic structure calculations. This advantage makes *p-d* models of (III,Mn)V ferromagnets particularly useful. *s-d* models of transition elements are less realistic from the start because they do not account for the minority-spin hybridized *s-d* bands which are present at the Fermi energy.

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[18] $C(1)$ and $C(\infty)$ differ by as much as 25%; the disparity between $B(1)$ and $B(\infty)$ may be even larger.

[19] The disorder dependence in α_G originates not only from the vertex part but also from the Green's functions as well. It is useful to recall that $\int G_\sigma G_{-\sigma} \propto 1/[b+i\mathrm{sg}(\sigma)\gamma]$ and $\int G_\sigma G_\sigma \propto 1/\gamma$.

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[21] Notwithstanding that the four-band model is a SO$\rightarrow\infty$ limit of the more general six-band model, we shall tune the effective spin-orbit strength via p (hole concentration) and γ_3.

[22] Strictly speaking, it is $|s^x_{\alpha,\beta}|^2 \simeq |K_{\alpha,\beta}|^2$ that is needed rather than $s^x_{\alpha,\beta} \simeq K_{\alpha,\beta}$. The former condition is less demanding and can occasionally be satisfied when $E_\alpha - E_\beta$ is on the order of the exchange splitting.