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 provides 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 $\alpha_G$ in current-driven and precessional 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\cite{Garcia08}. 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\cite{Parkin08} reported successful applications to transition metal ferromagnets of the torque-correlation formula\cite{vonOppen07,Imada98,Imada98b} for $\alpha_G$. This formula has the important advantage that its application requires knowledge only of the band structure, including its spin-orbit 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 (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\cite{Garcia08}. The self-consistent Born approximation theory for $\alpha_G$ requires that ladder-diagram vertex corrections be included in the transverse spin-spin response function. Since the Born approximation is exact 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 intra-band excitations of the transition metal Fermi sea, but that it can be inaccurate when it is dominated by inter-band excitations.

Our paper is organized as follows. In Section 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 Section IV summarizes our findings for the four-band (III,Mn)V model. We conclude in Section 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 vs. s-d and p-d models

We view the two-band $s-d$ and four bandwidth $p-d$ models studied in this paper as toy models which capture the essential features of metallic magnetism in systems that are, at least in principle, 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 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 we have proposed the following expression for the Gilbert-damping contribution from particle-hole excitations in SDFT bands:

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

(1)

where $\chi^{QP}_{x,x}$ 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,

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

(2)

where $\alpha$ and $\beta$ label the $x$ and $y$ transverse spin directions and the easy direction for the magnetization is assumed to be the $z$ direction. In Eq. (2) $|i\rangle$, $f_i$ and $\omega_{ij}$ are Kohn-Sham eigen-spinors, Fermi factors, and eigenenergy differences respectively, $s_\alpha$ is a spin operator, and
\[ \Delta_0(\vec{r}) \] is the difference between the majority spin and minority spin exchange-correlation potential. In the \( s - d \) and \( p - d \) models \( \Delta_0(\vec{r}) \) is replaced by a phenomenological constant, which we denote by \( \Delta_0 \) below. With \( \Delta_0(\vec{r}) \) replaced by a constant \( \chi_{xx}^{QP} \) reduces to a standard spin-response function for non-interacting quasiparticles in a possibly spin-dependent random static external potential. The evaluation of this quantity, and in particular the low-frequency limit in which we are interested, is non-trivial 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,

\[ \chi_{xx}^{QP}(i\omega) = -V\frac{\Delta_0^2}{\beta} \sum_{\omega_n} P(i\omega_n, i\omega_n + i\omega) \]  

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

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

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

\[ G_\alpha(i\omega_n, k) = \left[ i\omega_n + E_F - E_{k,\alpha} + i\frac{1}{2\tau_{k,\alpha}}\text{sign}(\omega_n) \right]^{-1}. \]

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

![FIG. 1: Dyson equation for the renormalized vertex of the transverse spin-spin response function. The dotted line denotes impurity scattering.](image)

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

\[ \Lambda_{\alpha,\beta}(i\omega_n, i\omega_n + i\omega; k) = s^x_{\alpha,\beta}(k) + \int \frac{d^Dk'}{(2\pi)^D} u^a(k - k') s^{a}_{\alpha,\alpha'}(k, k') G_{\alpha'}(i\omega_n, k') \Lambda_{\alpha',\beta'}(i\omega_n, i\omega_n + i\omega; k') G_{\beta'}(i\omega_n + i\omega, k') s^{a}_{\beta',\beta}(k', k), \]

where \( u^a(q) \equiv n_a V_a^2(q)(a = 0, x, y, z) \), \( n_a \) is the density of scatterers, \( V_a(q) \) is the scattering potential (dimensions: (energy) \( \times \) (volume)) and the overline stands for disorder averaging. Ward’s identity requires that

\[ u^a(q) \] and \( \tau_{k,\alpha} \) be related via the Fermi’s golden rule:

\[ \frac{1}{\tau_{k,\alpha}} = 2\pi \int k' u^a(k - k') \sum_{\alpha'} s^{a}_{\alpha,\alpha'} s^{a}_{\alpha',\alpha} \delta(E_{k\alpha} - E_{k'\alpha'}), \]

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

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

(8)

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

\[
\alpha_G = \frac{\Delta_0^2}{2\pi s_0} \left\{ \text{Re} \left[ P(-i\delta, i\delta) \right] - \text{Re} \left[ P(i\delta, +i\delta) \right] \right\}
\]

\[
= \frac{\Delta_0^2}{2\pi s_0} \text{Re} (P^{A,R} - P^{R,R})
\]  

(9)

where \( s_0 = S_0/V \),

\[
P^{R(A),R} = \int_k \Lambda_{\alpha,\beta}^{R(A),R}(k) G_{\beta}^R(0,k)s_{\beta,\alpha}(k) G_{\alpha}^R(0,k)
\]

(10)

and \( G_{\alpha}^R(0,k) \) 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 Sections III and IV to its application to the \( s-d \) and \( p-d \) models.

C. Evaluation of Impurity Vertex Corrections for Multi-Band Models

Eq.(9) 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.

\[
U_{m,m';i,l'}^{R(A),R} = (u^0 + u^z mm') \int_k \langle m|\alpha k|\langle m'|\alpha' k'\rangle s_{\alpha,\alpha'}^z(k)
\]

(13)

Eqs. (12), (13) and (14) provide a solution for the vertex function that is significantly easier to analyse than the original Dyson equation.

III. GILBERT DAMPING FOR A MAGNETIC 2DEG

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, 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 factors. 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, the Gilbert damping of a M2DEG has qualitative features similar to those of (Ga,Mn)As.

The band Hamiltonian of the M2DEG model is

\[ H = \frac{k^2}{2m} + b_k \cdot \sigma \]

(15)

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

\[ E_{\pm k} = \frac{k^2}{2m} \pm \sqrt{\Delta_0^2 + \lambda^2 k^2} \]

(16)

\[ |\alpha k\rangle = e^{-is^\alpha x} e^{-is^\alpha \theta} |\alpha\rangle \]

(17)

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

\[ \langle m|\alpha, k \rangle = \langle m|e^{-is^\alpha x}\phi e^{-is^\alpha \theta}|\alpha\rangle = e^{-im\phi} d_{m, \alpha}(\theta) \]

where \( d_{m, \alpha} = \langle m|e^{-is^\alpha \theta}|\alpha\rangle \) is a Wigner function for \( J=1/2 \) angular momentum. With these simple spinors, the azimuthal integral in Eq. (13) can be performed analytically to obtain

\[
U_{m, m'}^{R(A), R} \delta_{m'-\bar{m}, \bar{m}'} (u^0 + u^m m') \sum_{\alpha, \beta} \int \frac{d\mathbf{k} k}{2\pi^2} d_{m\alpha} G^R_{\alpha}(k) d_{\bar{m}'\beta}(\theta) G^R_{\bar{\alpha}}(k) d_{\bar{m}'\beta}(\theta),
\]

(19)

where the Kronecker delta reflects the conservation of the angular momentum along \( z \), owing to the azimuthal symmetry of the problem. In Eq. (13)

\[ d_{m, m'} = \left( \begin{array}{cc} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{array} \right), \]

(20)

and the retarded and advanced Green’s functions are

\[ G^R_{\alpha}(k) = \frac{1}{-\xi_k - b_k + (-i)\gamma}, \]

\[ G^A_{\alpha}(k) = \frac{1}{\xi_k + b_k + (-i)\gamma}, \]

(21)

where \( \xi_k = \frac{k^2 - \Delta_0^2}{2m} \), \( b_k = \sqrt{\Delta_0^2 + \lambda^2 k^2} \), and \( \gamma \) is (half)

\[
U_{\bar{m}, +; \bar{m}', -}^{R, R} = U_{+, +; +, +}^{R, R} = 0
\]

\[
U_{\bar{m}, +; \bar{m}', -}^{A, A} = (\gamma_0 - \gamma) \left[ \frac{i}{-b + i\gamma} \cos^4 \left( \frac{\theta}{2} \right) + \frac{i}{b + i\gamma} \sin^4 \left( \frac{\theta}{2} \right) + \frac{2}{\gamma} \cos^2 \left( \frac{\theta}{2} \right) \sin^2 \left( \frac{\theta}{2} \right) \right]
\]

(23)

where \( b \approx \sqrt{\lambda^2 k_F^2 + \Delta_0^2} \) and \( \cos \theta \approx \Delta_0/b \). The first and second terms in square brackets in Eq. (23) emerge from inter-band transitions \((\alpha \neq \beta)\) in Eq. (19), while the last term stems from intra-band transitions \((\alpha = \beta)\).

Amusingly, \( U \) vanishes when the spin-dependent scattering rate equals the Coulomb scattering rate \((\gamma_\perp = \gamma_0)\); in this particular instance vertex corrections are completely absent. On the other hand, when \( \gamma_\perp = 0 \) and \( b << \gamma \)
we have $U^{A,R}_{-\lambda,-} \simeq U^{A,R}_{-+} \simeq 1$, implying that vertex corrections strongly enhance Gilbert damping (recall Eq. (22)). We will discuss the role of vertex corrections more fully below.

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

$$P^{R(A),R}_{\alpha,\beta} = \int_k \Lambda^{R(A),R}_{\alpha,\beta}(k) s_{\beta,\alpha}^x(k) G^{R(A)}_\alpha(k) G^{R}_\beta(k).$$

(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 $P^{R,R}_{\alpha,\beta} \simeq 0$. In the case of spin-independent scatterers ($\gamma_z = 0 \rightarrow \gamma = \gamma_0$), tedious but straightforward algebra takes us to

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

(25)

Eq. (29) agrees with results published in the recent literature. 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 $b >> \gamma_0$ regime:

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

(26)

which displays intra-band ($\sim \gamma_0^{-1}$) and inter-band ($\sim \gamma_0$) contributions separately. The intra-band damping is due to the dependence of band eigenenergies on magnetization orientation, the breathing Fermi surface effect (which produces more damping when the band-quasiparticles scatter infrequently because the population distribution moves further from equilibrium. The intra-band contribution to damping therefore tends to scale with the conductivity. For stronger disorder, the inter-band term in which scattering relaxes spin-

FIG. 2: **M2DEG**: Gilbert damping in the absence of spin-orbit coupling. When the intrinsic spin-orbit interaction is small, the 1st vertex correction is sufficient for the evaluation of Gilbert damping, provided that the ferromagnet’s exchange splitting is large compared to the lifetime-broadening of the quasiparticle energies. For more disordered ferromagnets ($E_F \gamma_0 < 5$ in this figure) higher order vertex corrections begin to matter. In either case vertex corrections are significant. In this figure $1/\gamma_0$ 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 $u^0 = 3 u^z$.

FIG. 3: **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: **M2DEG**: Gilbert damping for moderate SO interactions ($\lambda k_F = 0.2 E_F \simeq 0.5 \Delta_0$). In this case there is a crossover between the intra-band dominated and the inter-band dominated regimes, which gives rise to a non-monotonic dependence of Gilbert damping on disorder strength. The stronger the intrinsic SO relative to the exchange field, the higher 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).
orientations takes over and $\alpha_G$ is proportional to the resistivity. Insofar as phonon-scattering can be treated as elastic, the Gilbert damping will often show a non-monotonic temperature dependence with the intra-band mechanism dominating at low-temperatures when the conductivity is large and the inter-band mechanism dominating at high-temperatures when the resistivity is large.

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

$$\alpha_G(u^0 = 0) \simeq \frac{N_{2D}}{2s_0} \frac{N_{2D}}{\Delta_0^2} \left[ \frac{1}{\gamma_z} \frac{1}{6b^2 - 2\Delta_0^2} + \frac{3b^4 + 6b^2\Delta_0^2 - \Delta_1^2}{(3b^2 - \Delta_0^2)^3} \right]$$

This expression illustrates that spin-orbit (SO) interactions in the band structure are a necessary condition for the intra-band transition contribution to $\alpha_G$. The interband contribution survives in 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 Eq. (26) and Eq. (27): in the former the inter-band coefficient is most suppressed at weak intrinsic SO interaction while in the latter it is the intra-band coefficient which gets weakest for small $\lambda k_F$.

More general cases relaxing the $(\Delta_0, \lambda k_F, \gamma) << E_F$ assumption must be studied numerically; the results are collected in Figs. (2), (3) and (4). Fig (2) highlights the inadequacy of completely neglecting vertex corrections in the limit of weak spin-orbit interaction; the inclusion of the the leading order vertex correction largely solves the problem. However, Fig. (2) and (3) together indicate that higher order vertex corrections are noticeable when disorder or spin-orbit coupling is strong. In the light of the preceding discussion the monotonic decay in Fig.(3) may appear surprising because the interband contribution presumably increases with $\gamma$. Yet, this argument is strictly correct only for weakly spin-orbit coupled systems, where the crossover between interband and intra-band 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 inter-band contribution behaves much like its intra-band partner, i.e. $O(1/\gamma)$. Non-monotonic 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, Shibata and Tatar claim that the bare vertex along with the first vertex correction fully captures the Gilbert damping of a ferromagnet, provided that $\Delta_0 \tau >> 1$. To first order in $U$ the vertex function is

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

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

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

$$A(1) \approx 1 \quad A(\infty)$$

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. (28) transforms into

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

$$B(1) = \frac{\Delta_0^2(3b^2 - \Delta_0^2)^3(3b^2 + \Delta_0^2)}{4b^6(3b^4 + 6b^2\Delta_0^2 - \Delta_1^2)}$$

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

When $\Delta_0 << \lambda k_F$, both intra-band and inter-band ratios show a significant deviation from unity, 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 $\Delta = \frac{1}{\gamma} \sum_{n=0}^{\infty} U^n$, where the $n$-th order term stems from the $n$-th vertex correction. From Eq. (28) 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 $O(\gamma^{12})$ when $E_F >> \gamma$. In contrast, when $\lambda \neq 0$ the intra-band term in Eq. (28) 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 “intra-band~ $O(1/\gamma)$; inter-band~ $O(\gamma)$”. Our expectation that higher order vertex corrections be important in (Ga,Mn)As will be confirmed numerically in the next section.

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 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 states 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 \( \alpha_G \) significantly at all orders; this is the central idea of this section.

Using a p-d mean-field theory model\(^{23} \) for the ferromagnetic ground state and a four-band spherical model\(^{1,9} \) for the host semiconductor band structure, Ga\(_{1-x}\)Mn\(_x\)As may be described by

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

where \( \mathbf{s} \) is the spin operator projected onto the \( J=3/2 \) total angular momentum subspace at the top of the valence band and \( \{ \gamma_1 = 6.98, \gamma_2 = \gamma_3 = 2.5 \} \) are the Luttinger parameters for the spherical-band approximation to GaAs. In addition, \( \Delta_0 = J_{pd} S N_{Mn} \) is the exchange field, \( J_{pd} = 55\text{meV}\text{nm}^3 \) is the p-d exchange coupling, \( S = 5/2 \) is the spin of the Mn ions, \( N_{Mn} = 4x/a^3 \) is the density of Mn ions, and \( a = 0.565\text{nm} \) is the lattice constant of GaAs.

The \( \Delta_0 = 0 \) eigenstates of this model are

\[
|\hat{\alpha}, \mathbf{k}\rangle = e^{-i\mathbf{s}^z \Phi} e^{-i\theta} |\hat{\alpha}\rangle \tag{32}
\]

where \( |\hat{\alpha}\rangle \) is an eigenstate of \( \mathbf{s}^z \) with eigenvalue \( \hat{\alpha} \). 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 \( \Phi \)-dependence of the full eigenstates \( |\alpha\rangle \) will be identical to that of Eq. (32). This observation leads to \( U_{m,m';\ell,\ell'} \propto \delta_{m-m',\ell-\ell'} \), which simplifies Eq. (14). \( \alpha_G \) can be calculated numerically following the steps detailed in the previous sections; 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. Fig. (5) underlines both the importance of higher order vertex corrections in \( \text{(Ga,Mn)As} \) and the monotonic decay of the damping as a function of scattering rate. The latter signals the supremacy of the intra-band contribution to damping, accentuated at larger hole concentrations.

Had the intrinsic spin-orbit interaction been substantially weaker, \( \alpha_G \) would have traced a non-monotonic 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 Figs. (3)-(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.

\[\text{FIG. 5: GaMnAs:} \text{ Higher order vertex corrections make a significant contribution to Gilbert damping, due to the prominent spin-orbit interaction in the band structure of GaAs.} \]

\[\text{FIG. 6: GaMnAs:} \text{ When the spin-orbit splitting is reduced (in this case by reducing the hole density to 0.2nm}^{-3} \text{ and artificially taking } \gamma_3 = 0.5, \text{ the crossover between inter- and intra-band dominated regimes produces a non-monotonic shape of the Gilbert damping, much like in Fig. (1). When either } \gamma_2 \text{ or } p \text{ is made larger or } x \text{ is reduced, we recover the monotonic decay of Fig. (6).} \]

\[\text{V. ASSESSMENT OF THE TORQUE-CORRELATION FORMULA} \]

Thus far we have evaluated the Gilbert damping for a M2DEG model and a \( \text{(Ga,Mn)As} \) model using the (bare) spin-flip vertex \( (\alpha, \mathbf{k})|s^z \beta\rangle \) and its renormalized counterpart \( (\alpha, \mathbf{k})|\Lambda|\beta\rangle \). 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\(^2 \) 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:\(^5\)

\[
\langle \alpha, \mathbf{k} | s^x | \beta, \mathbf{k} \rangle = \frac{i}{\Delta_0} (E_{k,\alpha} - E_{k,\beta}) \langle \alpha, \mathbf{k} | s^y | \beta, \mathbf{k} \rangle
\]

In Eq. (33) we have decomposed the mean-field quasi-particle Hamiltonian into a sum of spin-independent, exchange spin-splitting, and other spin-dependent terms: \( H = H_{\text{kin}} + H_{\text{so}} + H_{\text{ex}} \), where \( H_{\text{kin}} \) is the kinetic (spin-independent) part, \( H_{\text{ex}} = \Delta_0 s^x \) is the exchange spin-splitting term and \( H_{\text{so}} \) 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:

\[
\langle \alpha, \mathbf{k} | K | \beta, \mathbf{k} \rangle \equiv \frac{i}{\Delta_0} \langle \alpha, \mathbf{k} | H_{\text{so}} | \beta, \mathbf{k} \rangle. \tag{34}
\]

Eq. (34) allows us to make a few general remarks on the relation between the spin-flip and torque-correlation matrix elements. For intra-band matrix elements, one immediately finds that \( s^x_{\alpha,\alpha} = K_{\alpha,\alpha} \) and hence the two approaches agree. For inter-band 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 \( (E_{k,\alpha} - E_{k,\beta}) \ll \Delta_0 \). Since this requirement cannot be satisfied in the M2DEG, we expect that the inter-band contributions from \( K \) and \( s^x \) will always differ significantly in this model. More typical models, like the four-band model for (Ga,Mn)As, have band crossings at a discrete set of k-points, in the neighborhood of which \( K_{\alpha,\beta} \sim s^x_{\alpha,\beta} \). 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 \( \tau \) (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 inter-band contribution 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 non-perturbatively.\(^6\)

![FIG. 7: 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 (\( \lambda k_F = 0.05E_F \approx 0.06\Delta_0 \)) and we have taken \( u^z = 0 \). The torque correlation formula does not distinguish between spin-dependent and spin-independent disorder.](image)

![FIG. 8: 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 \( u^z = 0 \).](image)

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 \( \alpha_K \) analytically using \( K \) instead of \( s^x \) and neglecting vertex corrections; we obtain:

\[
\alpha_K = \frac{N_{2D}}{8s_0} \left[ \frac{\lambda^2 k_F^2}{b^2} \frac{\Delta_0}{\gamma} + \left( \frac{\lambda^2 k_F^2}{\Delta_0 b} \right)^2 \frac{\gamma \Delta_0}{\gamma^2 + b^2} \right] \tag{35}
\]
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 intra-band parts are in excellent agreement when \(\Delta_0 \ll \lambda k_F\), i.e., when vertex corrections are relatively unimportant. In contrast, the inter-band 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 \(\Lambda\) matrix elements. Fig. (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 inter-band contribution does not vanish even as SO tends to zero. As explained in Section 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 intra-band contributions dominate and therefore \(s^x\) and \(K\) coincide; even \(\Lambda\) agrees, because for intra-band transitions the vertex corrections are unimportant. Fig. (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 intra-band part substantially. For a similar reason, neither \(s^x\) nor \(K\) agree with the exact \(\Lambda\) 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 \(\alpha_G\) when spin-orbit interactions are strong and \(\alpha_G\) is dominated by inter-band relaxation. A precise estimation of \(\alpha_G\) 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 intra-band contributions accurately when the vertex corrections are unimportant, while it is less reliable for inter-band contributions unless the predominant inter-band 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 inter-band and intra-band contributions be evaluated separately when \(\alpha_G\) is evaluated using the torque-correlation formula. For the intra-band contribution the \(s^x\) and \(K\) life-time formulas are identical. The model calculations reported here sug-

![FIG. 9: GaMnAs: Comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex corrected result.](image)

![FIG. 10: GaMnAs: Comparison of Gilbert damping predicted using spin-flip and torque matrix element formulas, as well as the exact vertex corrected result.](image)
suggest that vertex corrections to the intra-band contribution do not normally have an overwhelming importance. We conclude that $\alpha_G$ can be evaluated relatively reliably when the intra-band contribution dominates. When the inter-band 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 splitting at the same wavevector. If the dominant contributions are from nearby bands, the damping estimate should have the same reliability as the intra-band contribution. If not, we conclude that the $\alpha_G$ estimate should be regarded with caution.

To summarize, this article 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 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 the supremacy of intra-band 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 \textit{ab-initio} calculations of the Gilbert damping is quantitatively reliable as long as the intra-band 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 life-time approximation formula offers no significant improvement over the original spin-flip matrix element.

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