Damping of near-adiabatic magnetization dynamics by excitations of electron-hole pairs

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Abstract. Excitation of electron hole pairs and subsequent relaxation is the most important mechanism of intrinsic damping in near-adiabatic magnetization dynamics in metallic ferromagnets. Intraband scattering dominates in the low temperature regime and is described by the breathing Fermi surface model. A Gilbert-like equation of motion is derived within this model where the constant damping scalar is replaced by a magnetization dependent and in general nonlocal damping matrix. In collinear systems the damping term shows two types of anisotropy, and in a general noncollinear situation nonlocal damping matrices enter the equation of motion.

1. Introduction
The investigation of ultrafast magnetization dynamics plays a key role in the development of future magnetic storage or information processing technologies. Therefore there has been an overwhelming interest during recent years to get a better understanding of the basic physical processes. Despite this effort, there are still enough open questions and we hope to answer some of them. The investigation of damping mechanisms in magnetization dynamics is especially important for controlable switching and reversal processes in magnetic devices.

Commonly, the phenomena of magnetization dynamics are subdivided into two groups according to the typical time scale they appear on. An example for the fs (femtosecond) time scale is the ultrafast demagnetization [1] of a ferromagnet after the excitation with a fs laser pulse. In this time regime strong excitations of the electronic ground state have to be taken into account. In contrast, in the near-adiabatic time regime of several ps (picoseconds) to ns (nanoseconds) the electronic system is assumed to be in its ground state with respect to the momentary orientations of the atomic magnetic moments [2]. Phenomena in this regime are the dynamics of domain walls [3] or field- and current-driven magnetization dynamics [3, 4].

In the near-adiabatic time regime, theoretical investigations are mostly micromagnetic simulations, which are based on the phenomenological Gilbert [5] equation for the magnetization $M(r,t)$,

$$\frac{dM}{dt} = -\gamma (M \times H_{\text{eff}}) + \frac{1}{M} M \times \alpha \frac{dM}{dt},$$

or on extensions which include the effect of spin polarized currents in current-driven dynamics. Here, $\alpha$ is the Gilbert damping scalar and $\gamma$ is the gyromagnetic ratio. The first term describes a precession of the magnetization around an effective field $H_{\text{eff}}$ and the damping term causes its
relaxation toward the equilibrium direction parallel to $H_{\text{eff}}$. In general, the effective field includes the magnetocrystalline anisotropy field, the exchange field, dipolar fields and the external field.

Now, the question arises if the description of damping through a rather simple damping term described by the constant damping scalar $\alpha$ is general enough to cope with complicated magnetic structures involving complicated magnetization trajectories.

Already Gilbert himself suggested [6] a more general damping term, which includes nonlocal damping matrices but couldn't represent them in an explicit way. In the breathing Fermi surface model [2, 7, 8, 9, 10], which we will introduce in the following section, an equation of motion can be derived [10], which includes such nonlocal damping matrices which additionally depend on the momentary configuration of the magnetization. The breathing Fermi surface model is valid in the near-adiabatic time regime, and it describes damping by the creation of electron hole pairs and subsequent relaxation through lattice scattering. The excitation of electron hole pairs and subsequent relaxation is the dominant [11] damping mechanism in metallic ferromagnets. We use the following section to explain the underlying physics of this mechanism, the role of the breathing Fermi surface model and the new equation of motion derived in this model. An overview about other damping mechanisms in magnetization dynamics is given in Ref. [12]. In section 3 the implications of the new equation of motion for collinear and noncollinear systems will be discussed.

2. Damping caused by excitation of electron hole pairs

To explain the physics underlying damping caused by the creation of electron hole pairs, we confine ourselves for the moment to a ferromagnetic collinear configuration. Then, the magnetization $\mathbf{M}(\mathbf{r}, t) = M_e(t)$ points throughout the sample into the same direction $\mathbf{e}(t)$. The magnitude $M$ of the magnetization is considered to be constant, so that the time dependence originates exclusively from the time dependent direction $\mathbf{e}(t)$. In a situation without external field and neglecting dipol effects, the magnetization will precess around the magnetocrystalline anisotropy field caused by spin orbit coupling.

When the direction of the magnetization evolves in time, the contribution of the spin orbit coupling energy gets time dependent. This time dependent spin orbit interaction excites electron hole pairs which have a finite lifetime. The relaxation of the electron hole pairs occurs through scattering at defects or phonons, where angular momentum and energy is transferred to the lattice system. The torque correlation model [13] and the breathing Fermi surface model describe this mechanism of magnetization damping. Both models treat the creation of electron hole pairs in an explicit way, whereas the subsequent relaxation is taken into account phenomenologically by a finite lifetime $\tau$ leading to lifetime broadening, or by a relaxation time $\tau$.

While the torque correlation model determines the damping parameter from the low-frequency limit of the transverse-spin-response function and its results are rather formal, the breathing Fermi surface model is based on an effective field approach. In order to give a physical more intuitive understanding of the torque correlation model, Gilmore et al. [14] recently managed to rederive the torque correlation formula in an effective field approach. In this approach, two types of electron hole pairs can be distinguished. The first type consists of an electron and a hole which occupy different energy bands, and it is generated when the time dependent spin orbit interactions excite transitions of single electrons into empty single electron states belonging to a different energy band. The contribution of this type of transitions to the torque correlation formula is called interband or bubbling Fermi surface contribution. In the second type of electron hole pairs, electron and hole occupy the same energy band and hence its contribution to the torque correlation formula is called intraband contribution. Gilmore et al. [14] showed in their effective field approach that this intraband contribution (also breathing Fermi surface contribution) is described by the breathing Fermi surface model. To understand the creation of electron hole pairs in this model, we define for a momentary direction $\mathbf{e}(t)$ of the...
magnetization at time $t$ the adiabatic single electron energies $\varepsilon_{jk}(e(t))$, where $j$ and $k$ denote the band index and the wavevector, the corresponding wavefunctions $\Psi_{jk}(e(t))$, the adiabatic Fermi Dirac occupation numbers $f_{jk}(e(t))$ and the adiabatic Fermi surface $S(e(t))$. All these quantities depend on the direction $e(t)$ via the spin orbit coupling and they change in time when $e(t)$ evolves in time. At time $t$ some single electron states which have been just below the Fermi level at time $t - dt$ get pushed above the Fermi energy, and others which have been just above at time $t - dt$ get pushed below. Now, we consider slightly nonadiabatic occupation numbers $n_{jk}(t)$ which lag behind the adiabatic Fermi Dirac occupation numbers $f_{jk}(t)$ because of the finite relaxation time $\tau$. Then, a state which was occupied at $t - dt$ can still be occupied at time $t$ although it would be empty in a strictly adiabatic situation and it represents an excited electron with respect to the adiabatic Fermi surface at time $t$. A hole is represented by a state which was unoccupied at time $t - dt$ and still is at time $t$ but would be occupied at time $t$ in an adiabatic situation.

The interband contribution shows a resistivity like temperature behaviour as it is proportional to the scattering rate $\tau^{-1}$, which means that it increases with increasing temperature and dominates in the high temperature regime [14]. The breathing Fermi surface contribution behaves conductivity like, as it is proportional to the inverse scattering rate $\tau$. So it dominates in the low temperature range and decreases with increasing temperature.

3. Breathing Fermi surface model in collinear and noncollinear systems

Now, that we have described the physical processes underlying the breathing Fermi surface model and explained the connection to the torque correlation model in a collinear system, we want to show results obtained for a general noncollinear situation. In Ref. [10] an equation of motion for the direction of the atomic magnetic moment $M_{R} = M_{R}e_{R}$ at site $R$ has been derived within the breathing Fermi surface model,

$$\frac{de_{R}}{dt} = -\gamma e_{R} \times H_{\text{eff},R}\{e_{R'}\} + e_{R} \times \sum_{R'} A_{R,R'}\{e_{R'}\} \cdot \frac{de_{R'}}{dt}. \quad (2)$$

The first term describes a precession around $H_{\text{eff},R}\{e_{R'}\}$, the effective field at the site $R$ which depends on the magnetic configuration $\{e_{R'}\}$ of the whole sample. The second term represents a Gilbert like damping term where the Gilbert damping scalar is replaced by a nonlocal configuration-dependent damping matrix $A_{R,R'}\{e_{R'}\}$. The damping matrices $A_{R,R'}$ depend on derivatives $\partial\varepsilon_{i}/\partial e_{R}$ of single electron energies with respect to the direction of the atomic magnetic moments,

$$A_{R,R'}\{e_{R'}\} = -\frac{\gamma}{} M_{R} \sum_{i} \frac{\partial f_{i}}{\partial e_{R}} \frac{\partial\varepsilon_{i}}{\partial e_{R}} \frac{\partial\varepsilon_{i}}{\partial e_{R'}}. \quad (3)$$

$\tau$ is the phenomenological relaxation time introduced by the breathing Fermi surface model and $f_{i}$ are the adiabatic Fermi-Dirac occupation numbers of single electron states. In principle, the relaxation time $\tau$ can be calculated by the ab-initio density functional electron theory, e.g., with Fermi’s golden rule. However, this would require to specify the scattering mechanism relevant for the specific material under consideration (e.g., scattering at phonons, defects, surfaces, grain boundaries, etc.). Because our theory is independent of the detailed scattering mechanism, it is natural to represent just the data for $A_{R,R'}/\tau$, as is done in Refs. [2, 8, 9, 10, 15, 16].

4. Implications of the new equation of motion and outlook

Equation (2) is a nonlocal equation of motion, which means that the damping at site $R$ depends on the time derivatives $de_{R'}/dt$ at the other sites $R'$. This feature is described by the nonlocal
damping matrices which have already been suggested by Gilbert in an abstract way, but now can be calculated. In this theory the origin of the nonlocality is the fact that single electron energies depend on the directions \{\epsilon_{\mathbf{R}'}\} of all atomic magnetic moments. It is only reasonable to use this property on a lengthscale where coherent single electron states exist. Because of this, only nonlocal damping matrices \(A_{\mathbf{R},\mathbf{R}'}\) for \(|\mathbf{R} - \mathbf{R}'|\) less than the electron mean free path are realistic. In the future we want to introduce a decay function which leads to a decrease on this characteristic length scale.

In a noncollinear system, the derivatives \(\partial e_i / \partial \epsilon_{\mathbf{R}}\) of single electron energies are dominated by exchange interactions, whereas in the collinear case they are caused by the relatively weak spin orbit coupling. Therefore, especially in strong canted configurations strong effects are expected.

In a collinear system, where all atomic magnetic moments are parallel to a common direction \(\mathbf{e} = \epsilon_{\mathbf{R}}\) for all \(\mathbf{R}\), eq. (2) reduces \cite{9} to an equation of motion for \(\mathbf{e}\).

\[
\frac{d\mathbf{e}}{dt} = -\gamma \mathbf{e} \times \mathbf{H}_{\text{eff}}(\mathbf{e}) + \mathbf{e} \times A(\mathbf{e}) \cdot \frac{d\epsilon}{dt}. \tag{4}
\]

The damping matrix \(A(\mathbf{e})\) has in general two different nonzero eigenvalues \cite{9,15}. These eigenvalues depend on the direction \(\mathbf{e}\) of the magnetization in the crystal via the spin orbit coupling \cite{9}. This represents the first of two types of anisotropy included in the damping term. The second type is given by the fact that the momentary damping depends on the momentary \(d\epsilon/dt\), because \(A(\mathbf{e})\) is a tensor. This effect is smeared out in FMR (ferromagnetic resonance) experiments, as there the trajectory of \(\mathbf{e}(t)\) is constrained to a precessional motion. The periodic change of \(d\epsilon/dt\) then averages over the generally different eigenvalues of \(A(\mathbf{e})\) \cite{16}.

Recent calculations in noncollinear systems have shown that the absolute values of the damping matrices \(A_{\mathbf{R},\mathbf{R}'}\) increase with increasing canting angles. This does not necessarily lead to increased damping. As one can see in eq. (2), the damping term at site \(\mathbf{R}\) depends not only on all damping matrices \(A_{\mathbf{R},\mathbf{R}'}\) but also on the dynamics \(d\epsilon_{\mathbf{R}'}/dt\). In very symmetric configurations and dynamics different contributions from sites \(\mathbf{R}'\) to the damping term at site \(\mathbf{R}\) can compensate each other. Further calculations will investigate the nonlocality in a noncollinear supercell. As described above, a decay function will be introduced into the theory to constrain the range of nonlocality to the lengthscale of the electron mean free path.

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