Generalized Gilbert equation including inertial damping: Derivation from an extended breathing Fermi surface model

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In a recent paper [M.-C. Ciornei *et al.*, Phys. Rev. B **83**, 020410(R) (2011)], it has been shown by mesoscopic nonequilibrium thermodynamics that, for relatively fast magnetization dynamics, Gilbert's equation of motion for the magnetization has to be supplemented by an "inertial" damping term that contains the second derivative of the magnetization with respect to time. In the present Brief Report, it is shown that such an additional damping term can be derived and evaluated very naturally also within a slightly extended breathing Fermi surface model for magnetization damping.

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In past years, there has been extensive research activity on dissipative magnetization dynamics. Thereby, the phenomena have been subdivided into fast and ultrafast magnetization dynamics. In the fast magnetization dynamics, the slow magnetic degrees of freedom are investigated on a time scale that is larger than the inverse of the frequencies ν of typical long-wavelength spin waves and hence much larger than the electronic intersite hopping time of about 10^{-15} s. For that time scale, the processes are close to the adiabatic limit for which the electronic system is always in its ground state with respect to the momentary magnetization configuration. Examples are the field- or spin-polarized-current-induced switching of the magnetization direction in films of several nm thickness or the switching of the polarization of a magnetic vortex core in a small platelet.[1] Ultrafast processes occur on shorter time scales, e.g., the quenching of ferromagnetic order in about 100 fs after exposing a thin film of Fe, Co, or Ni to an intense sub-100-fs pulse of laser light.[2]

On a phenomenological level, the fast near-adiabatic magnetization dynamics is often described by Gilbert's phenomenological equation[3] for the magnetization $\mathbf{M}(\mathbf{r},t)$,

$$\frac{d\mathbf{M}(\mathbf{r},t)}{dt} = -\gamma\ [\ \mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{\rm eff}(\mathbf{r},t)\ ] + \frac{1}{|\mathbf{M}(\mathbf{r},t)|}\left(\mathbf{M}(\mathbf{r},t) \times \alpha \frac{d\mathbf{M}(\mathbf{r},t)}{dt}\right). \quad (1)$$

Here the first term on the right-hand side (γ is the gyromagnetic ratio) describes the precession of the magnetization around the micromagnetic effective field $\mathbf{H}_{\rm eff}$, which is composed of the external field, the magnetic anisotropy field, and the demagnetization field. The second term is the damping term (with the damping number α), which drives the magnetization toward the direction of $\mathbf{H}_{\rm eff}$, whereby angular momentum is transferred to nonmagnetic degrees of freedom (direct damping).

Equation (1) is the simplest conceivable equation to describe near-adiabatic magnetization dynamics. The question is whether it is general enough to characterize the fast magnetization dynamics in all situations. It has been shown (see Refs. 4 and 5 and references therein) that even in the strict near-adiabatic regime the constant Gilbert damping number α in general has to be replaced by a nonlocal damping matrix $\underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'}$ that depends on the momentary orientations $\mathbf{e}_\mathbf{R}$ of the atomic magnetic moments $\mathbf{M}_\mathbf{R} = |\mathbf{M}_\mathbf{R}|\mathbf{e}_\mathbf{R}$ at all sites $\mathbf{R}$,

$$\frac{d\mathbf{e}_\mathbf{R}}{dt} = -\gamma\ \mathbf{e}_\mathbf{R} \times \mathbf{H}_{{\rm eff},\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}''}\}) + \mathbf{e}_\mathbf{R} \times \left(\sum_{\mathbf{R}'} \underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\}) \cdot \frac{d\mathbf{e}_{\mathbf{R}'}}{dt}\right). \quad (2)$$

The magnetization $\mathbf{M}(\mathbf{r},t)$ from Eq. (1) may be obtained from the atomic moments $\mathbf{M}_\mathbf{R}$,

$$\mathbf{M}(\mathbf{r},t) = \frac{1}{V(\mathbf{r})} \sum_{\mathbf{R}\in V(\mathbf{r})} \mathbf{M}_\mathbf{R}(t), \quad (3)$$

where $V(\mathbf{r})$ is the volume of a mesoscopic part of the sample around $\mathbf{r}$. Please note that, because of the replacement of α by the matrix $\underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'}$, the quantity $\underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'} \cdot (d\mathbf{e}_{\mathbf{R}'}/dt)$ in general is not parallel to $d\mathbf{e}_\mathbf{R}/dt$ on the left-hand side of Eq. (2). Other important consequences of the generalization of Gilbert's equation according to Eq. (2) are discussed in Ref. 4. The equation of motion (2) has been derived[4,5] by a combination of the effective-field theory (see below) of the breathing Fermi surface model[6] with a variant of the *ab initio* density functional electron theory based on the magnetic force theorem. The damping matrix $\underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'}$ could be represented in the form $\underline{\underline{\alpha}}_{\mathbf{R},\mathbf{R}'} = \tau\, \underline{\underline{f}}_{\mathbf{R},\mathbf{R}'}$, where τ is a relaxation time (see below) that covers in a lump sum all the electronic scattering processes that mediate the transfer of angular momentum from the spin system to the lattice and where $\underline{\underline{f}}_{\mathbf{R},\mathbf{R}'}$ depends only on the electronic structure and can be calculated by the *ab initio* density functional electron theory.

In past years, important experimental advances have been achieved, e.g., to speed up the above magnetization switching and to observe these processes with improved resolution in space and time (see, e.g., Ref. 7). The question arises how the equation of motion for the dynamics of $\mathbf{M}(\mathbf{r},t)$ has to be modified when leaving the strict near-adiabatic regime of the magnetization dynamics, i.e., when we want to describe the magnetization dynamics on the time scale of several ps or even a bit below (but not yet in the fs regime). In a recent paper

by Ciornei *et al.*,[8] this was investigated phenomenologically within the framework of mesoscopic nonequilibrium thermodynamics theory. Thereby a homogeneous magnetization $\mathbf{M}$ was considered, and the phase space of the ferromagnetic degrees of freedom was enlarged by the angular momentum of $\mathbf{M}$. Within this theory, a characteristic time τ_1 was introduced as a phenomenological parameter, and the behavior of the magnetization dynamics was separated in two regimes: the diffusion regime or the long time scale limit $t \gg \tau_1$, and the inertial regime $t \approx \tau_1$. In the diffusive regime, the equation of motion for $\mathbf{M}(t)$ has the form of Gilbert's equation with an inertial correction performed on the gyromagnetic ratio. For sufficiently short times $t \approx \tau_1$, however, the equation of motion [formulated with the constants γ and α of Gilbert's equation (1)] reads

$$\frac{d\mathbf{M}}{dt} = -\gamma\ (\mathbf{M} \times \mathbf{H}_{\text{eff}}) + \frac{1}{|\mathbf{M}|}\mathbf{M} \times \alpha \frac{d\mathbf{M}}{dt} + \frac{\alpha\tau_1}{|\mathbf{M}|}\mathbf{M} \times \frac{d^2\mathbf{M}}{dt^2}, \tag{4}$$

with a new "inertial"damping term determined by $d^2\mathbf{M}/dt^2$. It could be shown that this term generates a nutation loop superimposed to the usual Larmor-precession trajectory of $\mathbf{M}$ in a magnetic field.

It should be noted that this additional inertial damping term has been derived (among others) already by the theory of Suhl,[9] where the direct damping is described on a phenomenological level via the magnetoelastic coupling between the magnetization and the lattice distortions.

In the present Brief Report, we show that an additional damping term, which contains second time derivatives of $\mathbf{M}$, can be derived (among other additional terms) also within the framework of the above-mentioned effective-field theory of the breathing Fermi surface model. This derivation is very natural; it does not require the introduction of a new concept (like the angular momentum of $\mathbf{M}$) and it does not introduce a new parameter in addition to the one (the relaxation time τ) that determines α.

In the following, we consider also only the simple situation of a homogeneous magnetization. We define as strictly adiabatic situation the one for which the scattering processes of electrons are so fast and frequent that the electronic system is always in its ground state with respect to the orientation $\mathbf{e}(t)$ of the magnetization $\mathbf{M}(t) = M(t)\mathbf{e}(t)$. The orientation $\mathbf{e}(t)$ is the adiabatically slow magnetic degree of freedom[4,5,10] and plays the role of an external parameter for the electronic system. We then can define equilibrium single electron energies $\varepsilon_{j\mathbf{k}}[\mathbf{e}(t)]$, the corresponding single electron wave functions $\psi_{j\mathbf{k}}[\mathbf{e}(t)]$, the Fermi-Dirac occupation numbers $f_{j\mathbf{k}}[\mathbf{e}(t)]$, and the equilibrium Fermi surfaces $S[\mathbf{e}(t)]$. In a system with spin-orbit coupling, all these quantities change with $\mathbf{e}(t)$ in time, and as a result the Fermi surface breathes.

For a realistic, not strictly adiabatic but near-adiabatic situation, the electronic scattering processes are not able to produce at each moment an adiabatic equilibrium situation for the electronic system. If we knew the many-electron wave function $\Psi(t)$, we could calculate the homogeneous magnetization $\mathbf{M}(t)$ and hence its momentary orientation $\mathbf{e}(t)$. Knowing $\mathbf{e}(t)$, we could also calculate the adiabatic single-electron wave functions $\psi_{j\mathbf{k}}[\mathbf{e}(t)]$, and we could represent $\Psi(t)$ by the antisymmetrized product of the $\psi_{j\mathbf{k}}[\mathbf{e}(t)]$. However, the occupation numbers $n_{j\mathbf{k}}(t) = \langle\Psi(t)|\widehat{a}^+_{j\mathbf{k}}\widehat{a}_{j\mathbf{k}}|\Psi(t)\rangle$ will be different from the $f_{j\mathbf{k}}[\mathbf{e}(t)]$, where $\widehat{a}^+_{j\mathbf{k}}\widehat{a}_{j\mathbf{k}}$ is the particle number operator for the $\psi_{j\mathbf{k}}[\mathbf{e}(t)]$. The scattering processes will try to drive the $n_{j\mathbf{k}}(t)$ toward $f_{j\mathbf{k}}[\mathbf{e}(t)]$, but they will lag behind the $f_{j\mathbf{k}}[\mathbf{e}(t)]$.

It has been shown[4,5,10,11] that for a near-adiabatic situation the equation of motion for the orientation $\mathbf{e}(t)$ can be written in the form

$$\frac{d\mathbf{e}}{dt} = -\gamma\ \mathbf{e}(t) \times \widetilde{\mathbf{H}}_{\text{eff}}(t), \tag{5}$$

with the dissipative effective field,

$$\widetilde{\mathbf{H}}_{\text{eff}}(t) = -\frac{1}{M(t)}\frac{\delta E}{\delta \mathbf{e}(t)} = -\frac{1}{M(t)}\sum_{j\mathbf{k}} n_{j\mathbf{k}}(t)\frac{\partial \varepsilon_{j\mathbf{k}}[\mathbf{e}(t)]}{\partial \mathbf{e}(t)}, \tag{6}$$

where E is the total electronic energy. For the calculation of $n_{j\mathbf{k}}(t)$, a relaxation time ansatz is used (see also Ref. 6),

$$\frac{dn_{j\mathbf{k}}}{dt} = -\frac{1}{\tau_{j\mathbf{k}}}\{\, n_{j\mathbf{k}}(t) - f_{j\mathbf{k}}[\mathbf{e}(t)]\,\}. \tag{7}$$

A final approximation is to use just one relaxation time, $\tau_{j\mathbf{k}} = \tau$.

If $n_{j\mathbf{k}}$ at the arbitrary initial time t_0 is denoted as $n_{j\mathbf{k}}(t_0)$, then the formal solution of Eq. (7) can be written as

$$n_{j\mathbf{k}}(t) = \int_{t_0}^{t} \frac{1}{\tau} f_{j\mathbf{k}}(t') \exp\left(-\frac{t-t'}{\tau}\right) dt' + n_{j\mathbf{k}}(t_0)\exp\left(-\frac{t-t_0}{\tau}\right). \tag{8}$$

We now consider a dynamics for which $f_{j\mathbf{k}}[\mathbf{e}(t)]$ changes only slightly on the time scale τ, which determines the exponential decay terms, then it can be evaluated into a Taylor series around t. Neglecting transient solutions, i.e., for $(t - t_0) \to \infty$, this yields

$$n_{j\mathbf{k}}(t) = f_{j\mathbf{k}}[\mathbf{e}(t)] - \tau\ \frac{df_{j\mathbf{k}}}{dt}\bigg|_{\tau=0} + \tau^2\ \frac{d^2 f_{j\mathbf{k}}}{dt^2}\bigg|_{\tau=0} + \cdots. \tag{9}$$

The terms of higher order in τ are small corrections to the respectively preceding terms if the time scale $t_{\mathbf{e}}$ for the dynamics of $\mathbf{e}(t)$ and hence of $\varepsilon_{j\mathbf{k}}[\mathbf{e}(t)]$ is much larger than τ, $t_{\mathbf{e}}/\tau \gg 1$. In previous papers[4,5,10,11] on the near-adiabatic dynamics, the Taylor series (9) was terminated after the term linear in τ. We now consider a situation for which $t_{\mathbf{e}}/\tau$ is smaller, and we then take into account in Eq. (9) also the term quadratic in τ. Terms of the order τ^3 in Eq. (9) would yield additional damping terms, e.g., terms $\propto d^3\mathbf{e}/dt^3$, in analogy to third-order damping terms discussed by Suhl.[9]

To calculate the time derivatives of $f_{j\mathbf{k}}$, we must take into account that the Fermi-Dirac occupation numbers depend on the differences $\omega_{j\mathbf{k}}[\mathbf{e}(t)] = \varepsilon_{j\mathbf{k}}[\mathbf{e}(t)] - \mu[\mathbf{e}(t)]$ between the single-electron energies $\varepsilon_{j\mathbf{k}}[\mathbf{e}(t)]$ and the chemical potential $\mu[\mathbf{e}(t)]$, which is the Fermi energy $\varepsilon_F[\mathbf{e}(t)]$ for the case of zero temperature, i.e., $f_{j\mathbf{k}}[\mathbf{e}(t)] = f_{j\mathbf{k}}\{\,\omega_{j\mathbf{k}}[\mathbf{e}(t)]\}$; please

see the notes given in Ref. 12. With the chain rule, we then get

$$\frac{df_{j\mathbf{k}}}{dt} = \frac{\partial f_{j\mathbf{k}}}{\partial \omega_{j\mathbf{k}}}\left(\frac{\partial \omega_{j\mathbf{k}}}{\partial \mathbf{e}} \cdot \frac{d\mathbf{e}}{dt}\right), \tag{10}$$

$$\begin{aligned}\frac{d^2 f_{j\mathbf{k}}}{dt^2} = {} & \frac{\partial^2 f_{j\mathbf{k}}}{\partial \omega_{j\mathbf{k}}^2}\left(\frac{\partial \omega_{j\mathbf{k}}}{\partial \mathbf{e}} \cdot \frac{d\mathbf{e}}{dt}\right)^2 \\ & + \frac{\partial f_{j\mathbf{k}}}{\partial \omega_{j\mathbf{k}}}\left(\frac{\partial^2 \omega_{j\mathbf{k}}}{\partial \mathbf{e}^2} \cdot \frac{d\mathbf{e}}{dt}\right) \cdot \frac{d\mathbf{e}}{dt} \\ & + \frac{\partial f_{j\mathbf{k}}}{\partial \omega_{j\mathbf{k}}}\left(\frac{\partial \omega_{j\mathbf{k}}}{\partial \mathbf{e}} \cdot \frac{d^2\mathbf{e}}{dt^2}\right).\end{aligned} \tag{11}$$

In the second term on the right-hand side of Eq. (11), there is the product between the matrix $\partial^2 \omega_{j\mathbf{k}}/\partial \mathbf{e}^2$ and the vector $d\mathbf{e}/dt$, and then the dot product of the resulting vector with the vector $d\mathbf{e}/dt$. Inserting Eqs. (10) and (11) into Eq. (9) and then Eq. (9) into Eqs. (5) and (6) yields an equation of motion for $\mathbf{e}(t)$ with a damping term which is linear in de_i/dt [from Eq. (10)] and which has been reported already in Refs. 4, 5, and 10, and with additional damping terms [from Eq. (11)], one which is determined by $d^2 e_i/dt^2$ [from the last term of Eq. (11)], and others which contain products of $(de_i/dt) \cdot (de_j/dt)$ [from the first two terms of Eq. (11)]. e_i and e_j denote components of $\mathbf{e}$. Probably all three terms in Eq. (11) are relevant for the magnetization dynamics, but for the moment we consider only the last term of Eq. (11), arriving at

$$\frac{d\mathbf{e}}{dt} = -\gamma\, \mathbf{e} \times \mathbf{H}_{\text{eff}} + \mathbf{e} \times \left(\underline{\underline{\alpha}} \cdot \frac{d\mathbf{e}}{dt}\right) + \mathbf{e} \times \left(\underline{\underline{\alpha}}\tau \cdot \frac{d^2\mathbf{e}}{dt^2}\right), \tag{12}$$

with the microscopic expression for,

$$\mathbf{H}_{\text{eff}} = -\frac{1}{M}\sum_{j\mathbf{k}} f_{j\mathbf{k}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial \mathbf{e}}, \tag{13}$$

and with.

$$\frac{1}{\tau}\alpha_{m,n} = -\frac{\gamma}{M}\sum_{j\mathbf{k}} \frac{\partial f_{j\mathbf{k}}}{\partial \omega_{j\mathbf{k}}} \frac{\partial \omega_{j\mathbf{k}}}{\partial e_n} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_m}. \tag{14}$$

Note that $\underline{\underline{\alpha}}$ is not symmetric in m and n, in contrast to the former definition[4,5,10,11] of $\underline{\underline{\alpha}}$ where $\partial \omega_{j\mathbf{k}}/\partial e_n$ was replaced by $\partial \varepsilon_{j\mathbf{k}}/\partial e_n$; see Ref. 12. For a symmetric $\underline{\underline{\alpha}}$, one could replace in Eq. (12) $\underline{\underline{\alpha}}$ by $\alpha = \frac{1}{2} \cdot \text{Tr}(\underline{\underline{\alpha}})$ if the instantaneous $\mathbf{e}$ is parallel to a threefold or fourfold symmetry axis of the system.[10] All terms on the right-hand side of Eq. (12) are transverse to the instantaneous $\mathbf{e}$. This is a consequence of the fact that in the breathing-Fermi-surface model only $\mathbf{e}(t)$ is considered as an independent variable, whereas for $M(t)$ the value is used which corresponds to the equilibrium value for a system with fixed orientation $\mathbf{e}(t)$, i.e., $M(t)$ is slaved by $\mathbf{e}(t)$. Longitudinal terms (as in the Bloch equation) could only arise if the theory allowed for independent fluctuations of $M(t)$, i.e., for independent longitudinal fluctuations of $\mathbf{M}(t)$.

It should be noted that the damping terms in Eq. (12) are the consequence of a memory effect occurring for the time dependence of the magnetization in real systems. Such memory effects should occur in all real systems. The reason is that damping results from interactions of the spin degrees of freedom with other degrees of freedom, and from the time-dependent quantum-mechanical perturbation theory it becomes obvious that these interactions do not happen instantaneously but require time. On a phenomenological level, this has been emphasized already by Suhl.[9] In our microscopic theory, the memory effect appears in Eq. (8) for the occupation numbers $n_{j\mathbf{k}}$. We are convinced that each type of theory that takes into account memory effects will yield such damping terms. The value of our theory is that it allows one to represent these damping terms explicitly via the properties of the single-electron energies, which may be obtained from *ab initio* calculations. Thereby the theory is very general as long as time scales for $\mathbf{M}(t)$ are considered for which independent longitudinal fluctuations of $\mathbf{M}(t)$ can be neglected (see above). Then all possible interactions and electron scattering mechanisms are allowed that may be described by the use of just one relaxation time τ (for a critical discussion of this, see Ref. 13).

Equation (12) has the same basic form as Eq. (4), however, with the scalar quantity α replaced by the damping matrix $\underline{\underline{\alpha}}$. In the theory of Ref. 8, there are two parameters, α and τ_1, whereas in our theory there is just one parameter, the relaxation time τ. The complete right-hand side of Eq. (14) is given by the electronic structure of the system and can be calculated by the *ab initio* density functional electron theory. In Ref. 8, the parameter τ_1 has been introduced in a phenomenological manner to separate the diffusive part of the magnetization dynamics from the inertial part, but no microscopic meaning of τ_1 has been given. In our theory, the relaxation time τ has a well-defined microscopic meaning defined by Eq. (7). For their simulation of the precession-nutation behavior according to Eq. (4), the authors of Ref. 8 inserted $\tau_1 = 2$ ps and $\alpha = 5 \times 10^{-2}$. In Ref. 11, Fig. 2, the effective damping parameters α_{eff} for a basically circular precession of the magnetization are discussed as functions of τ^{-1}. For Ni and for the range of τ^{-1} values where the breathing Fermi surface damping dominates, values of α_{eff} between 0.2 and 0.01 are found for τ^{-1} ranging between 3×10^{12} s^{-1} and 10^{14} s^{-1}, i.e., the typical values of τ are smaller than $\tau_1 = 2$ ps used in Ref. 8. It would be interesting to repeat the simulation for a pair of values typical for Ni, e.g., $\alpha = 5 \times 10^{-2}$ and $\tau_1 = 0.1$ ps, in order to see how fast the Larmor precession must be in order that the nutation becomes remarkable.

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