### Breathing Fermi surface model for noncollinear magnetization: A generalization of the Gilbert equation

Manfred Fähnle\* and Daniel Steiauf

Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany (Received 20 December 2005; published 19 May 2006)

The breathing Fermi surface model which has been developed to describe the dissipative magnetization dynamics of collinear magnetization configurations is generalized to the case of noncollinear configurations. The theory is valid for small relative cantings of the atomic magnetic moments, and it is based on a phenomenological expansion of the *ab initio* density functional electron theory in atomic-sphere approximation for the spin direction. An equation of motion is obtained which looks like a Gilbert equation, with the important difference that Gilbert's damping constant is replaced by a damping matrix  $\alpha_{\mathbf{R}}(\{\mathbf{M_R}\})$  which in general is different for the different atomic sites  $\mathbf{R}$  and which depends on the momentary magnetization configuration  $\{\mathbf{M_R}\}$  of the whole system, i.e., it is a strongly nonlocal equation.

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#### I. INTRODUCTION

In the past few years there has been an intensive research activity to achieve a basic understanding of the ultrafast magnetization processes in magnetic materials, both experimentally and theoretically (for reviews, see Ref. 1). Among the various theoretical tools there are micromagnetic simulations for the dynamics of the magnetization field  $\mathbf{M}(\mathbf{r},t)$  which are mainly based on Gilbert's phenomenologically derived equation of motion<sup>2</sup>

$$\dot{\mathbf{M}}(\mathbf{r},t) = -\gamma \mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{\text{eff}}(\mathbf{r},t) + \frac{1}{M(\mathbf{r},t)} \mathbf{M}(\mathbf{r},t) \times \alpha \dot{\mathbf{M}}(\mathbf{r},t).$$
(1)

Here the first term describes a precessional dynamics where  $\gamma$  is the gyromagnetic ratio,  $\mathbf{H}_{\text{eff}}$  is the effective field which is composed<sup>3</sup> of the exchange field, the magnetic anisotropy field, the magnetic stray field, and the external field. The second term is Gilbert's damping term with the damping constant  $\alpha$ . Gilbert's equation is the simplest conceivable equation of motion for  $\mathbf{M}(\mathbf{r}, t)$ , and the question arises of course whether it is also a sufficiently general equation to describe magnetization dynamics in real magnets.

A physically intuitive microscopic approach to obtain an equation of motion for the atomic moments  $\mathbf{M}_{\mathbf{R}}(t)$  at the atomic sites  $\mathbf{R}$  is the breathing Fermi surface model.<sup>4–6</sup> It can be applied directly to magnetic 3*d* transition metals because it treats the electronic *s*, *p*, and *d* states on equal footing, and it can be combined with the highly accurate *ab initio* density functional electron theory.<sup>5,6</sup> So far it has been developed to describe magnetization damping in homogeneously magnetized systems. It thereby has been shown that even in this simple situation the original Gilbert equation does not hold but the damping scalar in Eq. (1) must be replaced by a damping matrix  $\underline{\alpha}(\mathbf{M})$  which depends on the momentary magnetization  $\mathbf{M}(t)$ .

In the present paper we extend the breathing Fermi surface model to noncollinear magnetization configurations. The motivation for this is twofold. First, in many physically and technologically interesting situations noncollinear configurations are involved (e.g., domain walls, magnetic vortices, inhomogeneous magnetization reversals, etc.). Second, within the breathing Fermi surface model the damping is related to the change of the shape of the Fermi surface originating from the temporal modification of the magnetic configuration. For a homogeneous magnet such a change arises exclusively from the spin-orbit coupling which in 3d metals is rather weak. For noncollinear situations the change arises in addition from the change of the exchange interactions which are much stronger than the spin-orbit couplings. We thus expect that the damping in noncollinear systems is stronger than the one in homogeneous systems.

#### **II. BASIC THEORY**

For a complete quantum-mechanical description of the dissipative magnetization dynamics one had to start from the time-dependent wave equation for electrons and nuclei, including spin-orbit coupling. Instead, we want to describe the situation approximately by an effective single-electron theory which involves only electrons and which describes the transfer of energy and angular momentum from the electrons to the nuclei via electronic scattering processes. It should be noted that (when dipolar effects are neglected) this transfer is only possible for a system with spin-orbit coupling. In such a theory the expectation values of observables are determined by the matrix elements of the respective operators formed with the single-electron spinor wave functions  $\psi_{i\mathbf{k}}(\mathbf{r},t)$  and by the occupation numbers  $n_{i\mathbf{k}}(t)$  describing the occupation of the states  $(j\mathbf{k})$  at time t. For instance, the spin magnetization density is given by

$$\mathbf{m}(\mathbf{r},t) = -\mu_B \sum_{j\mathbf{k}} n_{j\mathbf{k}}(t) \psi^*_{j\mathbf{k}s}(\mathbf{r},t) \hat{\boldsymbol{\sigma}}_{ss'} \psi_{j\mathbf{k}s'}(\mathbf{r},t), \qquad (2)$$

where  $\mu_B$  is Bohr's magneton and where  $\psi_{jks}$  is the *s* component of the spinor  $\psi_{jk}$  with band index *j* and wave vector **k**.

In principle, the  $\psi_{jk}(\mathbf{r},t)$  should be determined from the time-dependent single-electron wave equation. For a very

slow magnetization dynamics we can assume,<sup>7,8</sup> however, that the electronic system is at any instant in its ground state with respect to the momentary magnetic configuration  $\{\mathbf{e}_{\mathbf{R}}(t)\}$  given by the orientations  $\mathbf{e}_{\mathbf{R}}(t)$  of the atomic magnetic moments,

$$\mathbf{M}_{\mathbf{R}}(t) = M_{\mathbf{R}} \mathbf{e}_{\mathbf{R}}(t), \qquad (3)$$

at all sites **R**, and that the magnitudes  $M_{\mathbf{R}}$  are totally determined by this magnetic configuration. We thus may write

$$\psi_{j\mathbf{k}}(\mathbf{r},t) = \psi_{j\mathbf{k}}[\mathbf{r};\{\mathbf{e}_{\mathbf{R}}(t)\}],\tag{4}$$

$$\varepsilon_{i\mathbf{k}}(t) = \varepsilon_{i\mathbf{k}}[\{\mathbf{e}_{\mathbf{R}}(t)\}],\tag{5}$$

where the  $\varepsilon_{jk}$  are the single-electron energies, and

$$n_{j\mathbf{k}}(t) = f(\varepsilon_{j\mathbf{k}}[\{\mathbf{e}_{\mathbf{R}}(t)\}]) \equiv f_{j\mathbf{k}},\tag{6}$$

with the Fermi-Dirac equilibrium occupation numbers  $f_{ik}$ . All these quantities depend on the magnetic configuration  $\{\mathbf{e}_{\mathbf{R}}(t)\}\$  because of the spin-orbit coupling (which is the only source of theses dependencies for collinear magnetization configurations) and because of the exchange interactions (in the case of noncollinear systems). When changing  $\{e_R\}$  in time, the  $\psi_{i\mathbf{k}}$ ,  $\varepsilon_{i\mathbf{k}}$ ,  $n_{i\mathbf{k}}$ , the Fermi energy  $\varepsilon_F[\{\mathbf{e}_{\mathbf{R}}(t)\}]$ , and the Fermi surface will continuously attain a slightly different form ("breathing Fermi surface"). This so-called adiabatic approximation thereby assumes implicitly that the electronic system adjusts itself instantly to the new configuration  $\{\mathbf{e}_{\mathbf{R}}(t)\}\$  because the scattering processes of the electrons (at lattice defects or phonons) which are required for a redistribution of the occupation numbers appear on a time scale very much smaller than the characteristic time scale for the dynamics of the  $\mathbf{e}_{\mathbf{R}}(t)$ . Within this adiabatic approximation there is just a precessional dynamics of the magnetic moments without damping,<sup>9</sup>

$$\dot{\mathbf{e}}_{\mathbf{R}} = \mathbf{T}_{\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}'}\}),\tag{7}$$

where

$$\mathbf{T}_{\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}'}\}) = -\frac{2\mu_B}{\hbar} \frac{dE(\{\mathbf{e}_{\mathbf{R}'}\})}{d\mathbf{e}_{\mathbf{R}}} \times \mathbf{e}_{\mathbf{R}}$$
(8)

is the torque acting on the magnetic moment at site **R**, and *E* is the total energy which is a functional of the configuration  $\{\mathbf{e}_{\mathbf{R}'}\}$ .

The breathing Fermi surface model takes into account the fact that in reality the electronic scattering processes require a nonzero time. It is designed to describe a slightly nonadiabatic situation. Thereby it assumes that for the calculation of the expectation values of observables we can still use the adiabatic wave functions and eigenvalues, and that the deviation from the strictly adiabatic situation can be accounted for by inserting nonadiabatic occupation numbers  $n_{jk}$  which lag behind the  $f_{jk}$  and which are calculated from a relaxation ansatz

$$\frac{dn_{j\mathbf{k}}(t)}{dt} = -\frac{1}{\tau_{j\mathbf{k}}} [n_{j\mathbf{k}}(t) - f_{j\mathbf{k}}(t)]. \tag{9}$$

Here the  $\tau_{jk}$  are relaxation times which in general will depend on the electronic state (*j*k). For the case that  $\tau_{ik}$  is

much smaller than the characteristic time scale for the dynamics of the orientations  $\mathbf{e}_{\mathbf{R}}$ , the approximate solution of Eq. (9) is given by<sup>4-6</sup>

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$$i_{j\mathbf{k}}(t) = f_{j\mathbf{k}}(t) - \tau_{j\mathbf{k}} \frac{df_{j\mathbf{k}}(t)}{dt}.$$
 (10)

The scattering of the electrons at impurities or lattice vibrations thereby is responsible for the transfer of energy and angular momentum from the electrons to the lattice (via spinorbit coupling) and hence for the damping. With these assumptions a nonadiabatic total energy is defined, and the equation of motion is determined via Eqs. (7) and (8) with *E* replaced by  $E^{\text{nonad}}$ .

For the calculation of  $E^{\text{nonad}}$ , a phenomenological extension of the *ab initio* density functional electron theory is used.<sup>5,6</sup> In the strictly adiabatic limit, this theory yields two equivalent expressions for the total energy  $E[n, \{\mathbf{e}_{\mathbf{R}}(t)\}]$  for a given configuration  $\{\mathbf{e}_{\mathbf{R}}(t)\}$ , where  $n = (\rho[\mathbf{r}, \{\mathbf{e}_{\mathbf{R}}(t)\}]; \mathbf{m}[\mathbf{r}, \{\mathbf{e}_{\mathbf{R}}(t)\}]$  with the electronic density  $\rho$ ,

$$E = E_{\rm kin} + E_{\rm Hartree} + E_{\rm xc} + E_{\rm pot}, \qquad (11)$$

and

$$E = \sum_{j\mathbf{k}} n_{j\mathbf{k}} \varepsilon_{j\mathbf{k}} + E_{\mathrm{dc}}, \qquad (12)$$

where  $E_{\rm kin}$ ,  $E_{\rm Hartree}$ ,  $E_{\rm xc}$ ,  $E_{\rm pot}$ , and  $E_{\rm dc}$  denote the kinetic energy, the Hartree energy, the exchange correlation energy, the potential energy, and the double counting term, respectively. Because of the variational property of  $E(n, \{\mathbf{e_R}\})$  only those terms in Eq. (11) or Eq. (12) contribute to the derivative  $\partial E/\partial \mathbf{e_R}$  (and hence to the torque  $\mathbf{T_R}$ ) which depend explicitly (and not just implicitly via *n*) on the orientations  $\mathbf{e_R}$ .

## A. Collinear situation—the conventional breathing Fermi surface model

For homogeneously magnetized systems with spin-orbit coupling the double counting term  $E_{dc}$  in Eq. (12) depends only implicitly on the orientations of the magnetization via n, and therefore the torque  $\mathbf{T_R}=\mathbf{T}$  results exclusively from the first term in Eq. (12) where the  $\varepsilon_{j\mathbf{k}}$  (and hence also the  $n_{j\mathbf{k}}$ ) depend on the orientation of the magnetization in the crystal because of the spin-orbit coupling. Neglecting the dependence of the magnitude M of the magnetic moment  $\mathbf{M}=M\mathbf{e}$  on  $\mathbf{e}$ , as well as the dependence of  $\tau_{j\mathbf{k}}$  on  $(j\mathbf{k})$  the theory yields<sup>5,6</sup> the following equation of motion:

$$\dot{\mathbf{M}} = -\gamma \mathbf{M} \times \mathbf{H}_{aniso} + \frac{1}{M} \mathbf{M} \times \left[\underline{\alpha}(\mathbf{M}) \cdot \dot{\mathbf{M}}\right]$$
 (13)

with  $\gamma = -2\mu_B/\hbar$ . This equation looks very much like the Gilbert equation (1), with the only but very important difference that the constant damping scalar  $\alpha$  of the Gilbert equation is replaced by a matrix which depends on the orientation of **M**,

$$\frac{\alpha_{lm}}{\tau} = -\frac{\gamma}{M} \sum_{j\mathbf{k}} \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_l} \left| \begin{array}{c} \frac{\partial \varepsilon_{j\mathbf{k}}}{M} \\ M \end{array} \right|_{\mathbf{M}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_m} \right|_{\mathbf{M}}, \tag{14}$$

and the vector

$$\mathbf{H}_{\text{aniso}} = -\frac{1}{M} \sum_{j\mathbf{k}} f_{j\mathbf{k}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial \mathbf{e}}$$
(15)

is the anisotropy field. In Refs. 5 and 6 the quantities  $\partial \varepsilon_{j\mathbf{k}}/\partial \mathbf{e}$  are calculated by the *ab initio* density functional electron theory, using the transverse torque operator,<sup>10</sup> and the properties of the damping matrix  $\alpha$  are discussed. It turns out that for nanostructured materials like monolayers or monatomic wires the damping is identically zero for some orientations of **M**, and this represents an additional option for optimizing the magnetization reversal process in these nanostructures.

# B. Noncollinear situation—the modified breathing Fermi surface model

In this section we extend the breathing Fermi surface model to the case of noncollinear magnetization configurations. As described in the introduction, within this model the Fermi surface changes when changing the magnetization configuration. For noncollinear systems the change of the Fermi surface in general is dominated by the interatomic exchange interactions which are much stronger than the spinorbit interactions. The electronic system adjusts itself to a new magnetization configuration and hence to a new Fermi surface by scattering processes which require time and which transfer energy and angular momentum from the electrons to the lattice via spin-orbit coupling. Therefore, both for the homogeneous and for the noncollinear situation it is finally the spin-orbit coupling which is responsible for the damping, i.e., the exchange interactions on their own would not be able to generate damping. The difference between the two situations concerns only the "driving force" for damping, i.e., the change of the Fermi surface which is in general stronger for the noncollinear case. In the present section we therefore will neglect the spin-orbit coupling when calculating the change of the single-electron energies with configuration. The spinorbit coupling is included implicitly in the theory via the relaxation time ansatz for the occupation numbers  $n_{ik}$ .

To describe this situation, we will apply the so-called atomic-sphere approximation (ASA) for the spin direction.<sup>11,12</sup> To do this, the system is subdivided into space-filling atomic spheres of volume  $\Omega_{\mathbf{R}}$  at the atomic sites  $\mathbf{R}$ , and local spin quantization axes (SQAs) described by unit vectors  $\mathbf{e}_{\mathbf{R}}^{\text{SQA}}$  (with respect to which the Pauli spin matrices in the spheres are defined) are assigned to each atomic sphere. Then the local-spin-density approximation<sup>13</sup> (LSDA) for the exchange-correlation energy  $E_{xc}$ ,

$$E_{\rm xc}^{\rm LSDA} = \sum_{\mathbf{R}} \int_{\Omega_{\mathbf{R}}} \rho(\mathbf{r}) \varepsilon_{\rm xc} [\rho(\mathbf{r}), |\mathbf{m}(\mathbf{r})|] d^3 r, \qquad (16)$$

where  $\varepsilon_{xc}$  is the LSDA exchange-correlation energy per electron and  $|\mathbf{m}(\mathbf{r})|$  denotes the modulus of the magnetization density, is approximated by

$$E_{\rm xc}^{\rm ASA} = \sum_{\mathbf{R}} \int_{\Omega_{\mathbf{R}}} \rho(\mathbf{r}) \varepsilon_{\rm xc} [\rho(\mathbf{r}), \mathbf{e}_{\mathbf{R}}^{\rm SQA} \cdot \mathbf{m}(\mathbf{r})] d^3r.$$
(17)

The introduction of the spin ASA breaks the rotational invariance of the original LSDA exchange-correlation func-

tional (16), because now the exchange-correlation field  $\mathbf{B}_{\mathrm{xc}}^{\mathrm{ASA}} = -\delta E_{\mathrm{xc}}^{\mathrm{ASA}} / \delta \mathbf{m}(\mathbf{r})$  is parallel to  $\mathbf{e}_{\mathbf{R}}^{\mathrm{SQA}}$  in each atomic sphere and favors an orientation  $\mathbf{e}_{\mathbf{R}}$  of the atomic magnetic moment  $\mathbf{M}_{\mathbf{R}}$  close to  $\mathbf{e}_{\mathbf{R}}^{\text{SQA}}$  for the case that the  $\mathbf{e}_{\mathbf{R}}^{\text{SQA}}$  are noncollinear (for a collinear system we have  $\mathbf{e}_{\mathbf{R}} \equiv \mathbf{e}_{\mathbf{R}}^{\text{SQA}}$ ). On the other hand, the kinetic energy  $E_{\rm kin}$  favors a collinear magnetization density, and the competition between  $E_{\rm xc}$  and  $E_{\rm kin}$  results in misalignment angles  $\Delta \vartheta_{\rm R}$  between the  ${\bf e}_{\rm R}^{\rm SQA}$ and the  $\mathbf{e}_{\mathbf{R}}$  obtained for a density functional calculation in spin ASA. Because the  $B_{xc}^{ASA}$  are often large, the hope is that the  $\Delta \vartheta_{\mathbf{R}}$  are often small and that the directions  $\mathbf{e}_{\mathbf{R}}$  are to a good approximation given by the  $\mathbf{e}_{\mathbf{R}}^{\text{SQA}}$ . If this holds, then we can generate the noncollinear configurations  $\{e_R\}$  by prescribing the respective orientations  $\{e_{R}^{SQA}\}$ . It has been shown in Ref. 14 that this approximate constraining scheme for the directions  $\mathbf{e}_{\mathbf{R}}$  of the atomic magnetic moments may fail badly for the case of strong relative cantings of neighboring atomic moments. For small cantings, e. g., for a frozen-magnon configuration with a small cone-opening angle  $\vartheta$  and wave vector **q** the misalignment angles scale like<sup>12</sup>  $\Delta \vartheta_{\mathbf{R}} / \vartheta$  $\sim \omega(\mathbf{q})/|\langle \mathbf{B}_{xc} \rangle|$  where  $\langle \mathbf{B}_{xc} \rangle$  is an appropriately averaged exchange-correlation field and  $\omega(\mathbf{q})$  is the frequency of the magnon. For Fe with large  $|\langle \mathbf{B}_{xc} \rangle|$  this yields  $\Delta \vartheta_{\mathbf{R}} / \vartheta < 10\%$ whereas for Ni values of up to 46% were found for large q.

In the following we confine ourselves to situations where the above described constraining scheme for the atomic moment directions  $\{\mathbf{e_R}\}$  via the prescription of the  $\{\mathbf{e_R}^{ASA}\}$  for the exchange-correlation energy works reasonably well, and a necessary precondition for this is that we consider situations with small relative cantings of the atomic moments.<sup>14</sup> For a calculation of the derivatives  $\partial E/\partial \mathbf{e_R} \approx \partial E/\partial \mathbf{e_R}^{SQA}$  it is then convenient to start from Eq. (11), because the only term which depends explicitly on the orientations of the SQAs is  $E_{xc} = E_{xc}^{ASA}$ , Eq. (17). The kinetic energy  $E_{kin}$  does not depend explicitly on the  $\mathbf{e_R}^{SQA}$  because we neglect the spin-orbit coupling, and  $E_{Hartree}$  depends only implicitly via  $\rho$  on the  $\mathbf{e_R}^{SQA}$ . Taking again into account the variational property of E, the torque  $\mathbf{T_R}$  then is given by<sup>15</sup>

$$\mathbf{T}_{\mathbf{R}} = \frac{\partial E^{\mathrm{ASA}}}{\partial \mathbf{e}_{\mathbf{R}}} \times \mathbf{e}_{\mathbf{R}}$$
(18)

with

$$\frac{\partial E^{\text{ASA}}}{\partial \mathbf{e}_{\mathbf{R}}} = \mathbf{H}_{\text{ex},\mathbf{R}} = \frac{1}{2} \int_{\Omega_{\mathbf{R}}} \mathbf{m}_{\perp}(\mathbf{r}) [V_{\text{xc},\uparrow}(\mathbf{r}) - V_{\text{xc},\downarrow}(\mathbf{r})] d^3 r.$$
(19)

To derive Eq. (19), a spin-density matrix  $\rho_{ss'}$  is defined with respect to the local SQA (which represents the local z axis) by

$$\rho_{ss'}(\mathbf{r},t) = \sum_{j\mathbf{k}} n_{j\mathbf{k}}(t) \psi_{j\mathbf{k}s}^*(\mathbf{r},t) \psi_{j\mathbf{k}s'}(\mathbf{r},t), \qquad (20)$$

with  $\rho = \rho_{\uparrow\uparrow} + \rho_{\downarrow\downarrow}$ . The exchange-correlation potentials  $V_{\text{xc},\uparrow}$  and  $V_{\text{xc},\downarrow}$  then are given by

$$V_{\mathrm{xc},\uparrow}(\mathbf{r}) = \frac{\partial(\rho\varepsilon_{\mathrm{xc}})}{\partial\rho_{\uparrow\uparrow}}, \quad V_{\mathrm{xc},\downarrow}(\mathbf{r}) = \frac{\partial(\rho\varepsilon_{\mathrm{xc}})}{\partial\rho_{\downarrow\downarrow}}.$$
 (21)

The vector  $\mathbf{m}_{\perp}(\mathbf{r})$  is the component of the magnetization vector perpendicular to the SQA, with

$$\mathbf{m}_{\perp,x}(\mathbf{r}) = \rho_{\downarrow\uparrow}(\mathbf{r}) + \rho_{\uparrow\downarrow}(\mathbf{r}), \quad \mathbf{m}_{\perp,y}(\mathbf{r}) = -i\rho_{\downarrow\uparrow}(\mathbf{r}) + i\rho_{\uparrow\downarrow}(\mathbf{r}).$$
(22)

Altogether, we see that the torque  $\mathbf{T}_{\mathbf{R}}$  is a functional of the spin-density matrix, and in the strictly adiabatic limit we must insert the adiabatic occupation numbers  $n_{j\mathbf{k}}(t)$  given by Eq. (6), yielding  $\mathbf{T}_{\mathbf{R}} = \mathbf{T}_{\mathbf{R}}[\rho_{ss'}^{ad}(\mathbf{r})]$ .

To describe the slightly nonadiabatic situation, we again use a phenomenological extension of the *ab initio* density functional electron theory in the spirit of the breathing Fermi surface model. To do this we replace the torque  $\mathbf{T}_{\mathbf{R}}[\rho_{ss'}^{\mathrm{ad}}(\mathbf{r})]$ by the torque  $\mathbf{T}_{\mathbf{R}}^{\mathrm{nonad}} \equiv \mathbf{T}_{\mathbf{R}}[\rho_{ss'}^{\mathrm{nonad}}(\mathbf{r})]$  where the nonadiabatic spin-density matrix is calculated from Eq. (20) by inserting the adiabatic occupation numbers by the nonadiabatic occupation numbers given by Eq. (10). Evaluating  $\mathbf{T}_{\mathbf{R}}^{\mathrm{nonad}}$ around  $f_{j\mathbf{k}}$  up to first order in  $\tau_{j\mathbf{k}}$  and writing  $\partial f_{j\mathbf{k}}/\partial t$  in the form

$$\frac{\partial f_{j\mathbf{k}}}{\partial t} = \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial \mathbf{e}_{\mathbf{R}}} \dot{\mathbf{e}}_{\mathbf{R}}$$
(23)

and assuming again that  $\tau_{i\mathbf{k}} = \tau$  for all states  $(j\mathbf{k})$  we find

$$\mathbf{T}_{\mathbf{R}}^{\text{nonad}} = \mathbf{T}_{\mathbf{R}} + \mathbf{T}_{\mathbf{R}}^{\text{diss}}$$
(24)

with

$$\mathbf{T}_{\mathbf{R}}^{\text{diss}} = \mathbf{e}_{\mathbf{R}} \times \underline{\alpha}_{\mathbf{R}} \dot{\mathbf{e}}_{\mathbf{R}}$$
(25)

and with the damping matrix

$$\frac{\alpha_{pq,\mathbf{R}}}{\tau} = \sum_{j\mathbf{k}} \frac{\partial \mathbf{H}_{\text{ex},\mathbf{R},p}}{\partial n_{j\mathbf{k}}} \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \frac{\partial \varepsilon_{j\mathbf{k}}(\{\mathbf{e}_{\mathbf{R}'}\})}{\partial \mathbf{e}_{\mathbf{R},q}}.$$
 (26)

Because our theory holds only for small relative spin cantings (because we have used the spin ASA for constraining the moment directions) we can neglect again the dependence of the magnitudes  $M_{\mathbf{R}}$  of the magnetic moments  $\mathbf{M}_{\mathbf{R}} = M_{\mathbf{R}}\mathbf{e}_{\mathbf{R}}$  on the magnetic configuration  $\{\mathbf{e}_{\mathbf{R}'}\}$ , and then the equation of motion for the atomic moments  $\mathbf{M}_{\mathbf{R}}$  is

$$\dot{\mathbf{M}}_{\mathbf{R}} = -\gamma \mathbf{M}_{\mathbf{R}} \times \mathbf{H}_{\mathrm{ex},\mathbf{R}} + \frac{1}{M_{\mathbf{R}}} \mathbf{M}_{\mathbf{R}} \times \left[\underline{\boldsymbol{\varphi}}_{\mathbf{R}}(\{\mathbf{M}_{\mathbf{R}}\}) \cdot \dot{\mathbf{M}}_{\mathbf{R}}\right].$$
(27)

This equation has the same structure as the corresponding equation (13) for the case of a homogeneous magnetization, with the homogeneous variable **M** of (13) replaced by the site-resolved atomic moment  $\mathbf{M}_{\mathbf{R}}$  and with the anisotropy field  $\mathbf{H}_{aniso}$  of (15) replaced by the site-resolved exchange field  $\mathbf{H}_{ex,\mathbf{R}} = \partial E^{ASA} / \partial \mathbf{e}_{\mathbf{R}}$  according to Eq. (19).

### **III. DISCUSSION AND CONCLUSIONS**

Both the damping in homogeneous magnets as well as the in noncollinear systems are described by a damping term in the equation of motion which looks similar to the Gilbert damping term, however, with several important differences. First, the damping scalar  $\alpha$  of the Gilbert equation is replaced by a damping matrix which means that the damping term is no longer a vector perpendicular to the time derivative of the local magnetic moment. Second, the damping matrix depends in the magnetic configuration, in contrast to Gilbert's damping scalar. For homogeneous situations this configuration is described by the orientation of the magnetization,  $\alpha = \alpha(\mathbf{M})$ , whereas for noncollinear systems it is described by the orientations of all atomic magnetic moments in the system, i.e.,  $\alpha_{\mathbf{R}} = \alpha_{\mathbf{R}}(\{\mathbf{M}_{\mathbf{R}'}\})$ . As a result, for noncollinear systems the Gilbert equation which is a local equation is replaced by a nonlocal equation, i.e., the mathematical character of the equation of motion has been changed completely. Finally, in noncollinear magnets the damping matrix  $\alpha_{\mathbf{R}}$  is different for different sites **R** if the magnetic configurations in the surroundings are different for different **R**. This means that at least for systems for which the degree of relative cantings of magnetic moments is different for different parts of the system (e.g., very high in the core of a magnetic vortex and much smaller outside) it does not make sense to use just one damping matrix.

In the breathing Fermi surface model the damping matrix is determined by the dependence of the effective singleelectron energies on the modification of the magnetic configuration, and by the electronic scattering processes which transfer angular momentum from the electronic spin system to the lattice. The latter process is mediated by the spin-orbit coupling. The change of the single-particle energies results exclusively from the spin-orbit coupling for a homogeneously magnetized system, whereas in general there is a strong additional contribution from the exchange interactions for a noncollinear magnetization configuration. An exception is the case of a propagating spin wave. Because the exchange energy of a spin wave does not depend on its phase, the only dependence of the single-electron energies on the phase arises from the spin-orbit coupling.

There is another important difference between damping in a homogeneous system and in a noncollinear system. In the former case the damping matrix, Eq. (14), is of second order in the derivatives of the single-particle energies, whereas in the latter case it is of first order, see Eq. (26), like the magnetic anisotropy field  $\mathbf{H}_{aniso}$ , Eq. (15). Because the derivatives may be positive and negative for different electronic states  $(i\mathbf{k})$  there may be a near-cancellation of many terms in the sum over  $(j\mathbf{k})$  which may result in a delicate convergence behavior with respect to the number of considered states (as for  $\mathbf{H}_{aniso}$ ). However, it must be recalled that the derivatives are in general considerably larger for a noncollinear than for a collinear situation because the exchange coupling is stronger than the spin-orbit coupling. It is planned to figure out the relative importance of the two damping mechanisms by *ab initio* calculations for various representative situations.

To conclude, we have generalized the breathing Fermi surface model to the case of slightly noncollinear magnetization configurations. The damping term in the equation of motion has a similar structure as the Gilbert damping term, with the important difference that Gilbert's damping scalar is replaced by a damping matrix which in general is different for each atomic site and which depends in the whole magnetic configuration of the system, i. e., the resulting equation of motion is strongly nonlocal. For strongly noncollinear magnetization configurations (e. g., magnetic vortices of narrow domain walls) our detailed theoretical approach cannot be used, but we are convinced that also in such situations the general statements on the site dependence and the nonlocality of the damping term are valid. In addition, for such configurations not only the orientations  $\mathbf{e}_{\mathbf{R}}$  but also the magnitudes  $M_{\mathbf{R}}$  of the atomic magnetic moments  $\mathbf{M}_{\mathbf{R}}=M_{\mathbf{R}}\mathbf{e}_{\mathbf{R}}$  depend<sup>8</sup> on the whole magnetic configuration  $\{\mathbf{M}_{\mathbf{R}'}\}$  whereas in the Gilbert equation the magnitudes of the magnetic moments are conserved. Altogether, we must conclude that the Gilbert equation represents at most a very rough approximation for the equation of motion for noncollinear magnetization configurations.

\*Electronic address: faehnle@mf.mpg.de

- <sup>1</sup>Spin Dynamics in Confined Magnetic Structures I and II, edited by B. Hillebrands and K. Ounadjela (Springer, Berlin, 2003).
- <sup>2</sup>T. L. Gilbert, Ph.D. thesis, Illinois Institute of Technology, Chicago, 1956.
- <sup>3</sup>H. Kronmüller and M. Fähnle, *Micromagnetism and the Microstructure of Ferromagnetic Solids* (Cambridge University Press, Cambridge, 2003).
- <sup>4</sup>V. Kamberský, Can. J. Phys. **48**, 2906 (1970).
- <sup>5</sup>J. Kuneš and V. Kamberský, Phys. Rev. B **65**, 212411 (2002); **68**, 019901(E) (2003).
- <sup>6</sup>D. Steiauf and M. Fähnle, Phys. Rev. B **72**, 064450 (2005).
- <sup>7</sup>B. L. Gyorffy, A. J. Pindor, J. Staunton, G. M. Stocks, and H. Winter, J. Phys. F: Met. Phys. **15**, 1337 (1985).
- <sup>8</sup>R. Drautz and M. Fähnle, Phys. Rev. B **69**, 104404 (2004); M. Fähnle, R. Drautz, R. Singer, D. Steiauf, and D. V. Berkov,

Comput. Mater. Sci. 32, 118 (2005).

- <sup>9</sup>V. P. Antropov, M. I. Katsnelson, B. N. Harmon, M. van Schilfgaarde, and D. Kusnezov, Phys. Rev. B **54**, 1019 (1996); S. V. Halilov, H. Eschrig, A. Y. Perlov, and P. M. Oppeneer, *ibid.* **58**, 293 (1998).
- <sup>10</sup>X. Wang, R. Wu, D. S. Wang, and A. J. Freeman, Phys. Rev. B 54, 61 (1996).
- <sup>11</sup>J. Kübler, K. Höck, J. Sticht, and A. R. Williams, J. Phys. F: Met. Phys. **18**, 469 (1988).
- <sup>12</sup>O. Grotheer, C. Ederer, and M. Fähnle, Phys. Rev. B **62**, 5601 (2000).
- <sup>13</sup>U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
- <sup>14</sup>R. Singer, M. Fähnle, and G. Bihlmayer, Phys. Rev. B **71**, 214435 (2005).
- <sup>15</sup>O. Grotheer and M. Fähnle, Phys. Rev. B **59**, 13965 (1999).