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# Unified theory of near-adiabatic magnetization dynamics for collinear and noncollinear magnetization

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A combination of the breathing Fermi-surface model with a variant of the *ab initio* density-functional electron theory given by the magnetic force theorem is used to establish a unified theory for the near-adiabatic magnetization dynamics on the atomic scale. The main achievement of the theory is that it makes possible to treat both collinear as well as noncollinear magnetization configurations on equal footing. The theory yields an equation of motion of the type of the widely used Gilbert equation, however, with the constant Gilbert damping scalar replaced by an anisotropic and nonlocal damping matrix. The range of validity of the theory is discussed.

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In recent years, the ultrafast magnetization dynamics in magnetically ordered materials has been studied very extensively, both experimentally and theoretically.[1–9] From the viewpoint of fundamental research, this issue is very demanding because the coupling of the electronic system to the lattice has to be taken into account for dissipative spin dynamics. Technologically the issue is also of great importance for ultrafast switching of magnetic devices often formed by nanostructured systems. It has become customary to subdivide the phenomena into those which appear for time scales of say more than several picoseconds and those on the subpicosecond to femtosecond time scale. For the first situation (near-adiabatic situation) it is assumed that the electronic system is always close to its ground state with respect to the momentary magnetization configuration. Examples include the dynamics of domain walls[9] or the field- or current-induced magnetization dynamics in nanostructures.[1,9] For the second situation, strong electronic excitations from these ground states have to be taken into account, and an example is the ultrafast demagnetization by femtosecond[2] lasers. A first attempt to unify the phenomena on these two time scales was made by Koopmans *et al.*[3]

In the present Rapid Communication, we consider the first of the above discussed situations. Experiments on that time scale may be subdivided into those with a homogeneous collinear magnetization (such as the switching of small particles by coherent rotation or ferromagnetic resonance experiments) and those which involve nonuniform noncollinear magnetization configurations (such as domain walls or vortices). One very successful model for the explanation of dissipative magnetization dynamics on that time scale is the breathing Fermi-surface model introduced by Kambersky[4] already in 1970 and recast for collinear magnetization into a form which can be used in the *ab initio* density-functional theory much later.[5,6] In Ref. 7 a breathing Fermi-surface model for noncollinear situations has been suggested, because of the overwhelming importance of noncollinear magnetization configurations in technologically relevant magnetic devices, and because it is expected that the damping is much larger than in collinear systems (see below). The strategies to realize the breathing Fermi-surface model in the framework of the density-functional theory were, however, substantially different for collinear and noncollinear situations and therefore it is not clear whether the two situations were described on equal footing. Furthermore, in the former papers on the *ab initio* breathing Fermi-surface model, the orientations of the magnetic moments were prescribed only approximately via the local spin-quantization axes of the atomic-sphere approximation for the spin direction (spin ASA), and this is a good approximation for systems with weak noncollinearity and strong exchange-correlation fields only. In the present Rapid Communication, a unified approach will be presented which allows treating both situations on equal footing, and this is the main achievement of the unified theory. Furthermore, it refrains from the use of the spin ASA so that it can be applied also to the strongly noncollinear systems which appear frequently in modern nanoscale systems. This approach can serve as a general and firm basis for the discussion of near-adiabatic dissipative magnetization dynamics. The theory will predict an equation of motion (EOM) for atomic magnetic moments with an anisotropic and nonlocal damping term.

For a complete quantum-mechanical description of magnetization dissipation, i.e., of the transfer of angular momentum and heat from the electronic spin systems to the lattice, one had to start from the time-dependent wave equation for electrons and nuclei, involving spin-orbit coupling which mediates this transfer. Instead, we will describe the situation by an effective single-electron theory that involves only electrons and that describes the transfer empirically via scattering of electrons and a relaxation-time ansatz for the development of the electronic occupation numbers in time. Furthermore, for a near-adiabatic situation we consider only the slow magnetic degrees of freedom on a time scale which is larger than the inverse of the frequency $\nu$ of a typical long-wavelength spin wave. Then it is customary to define[8,10] atomic magnetic moments $\mathbf{M_R}=M_\mathbf{R}\mathbf{e_R}$ at the atomic sites $\mathbf{R}$ with magnitudes $M_\mathbf{R}$ and orientations $\mathbf{e_R}$ by integrating the electronic spin magnetization $\mathbf{m}(\mathbf{r},t)$ over the atomic sphere at site $\mathbf{R}$, respectively, and by averaging over the time $1/\nu$.

In a strictly adiabatic situation, the electronic scattering processes are so frequent that the electronic system follows the configuration $\{\mathbf{e_R}(t)\}$ of all magnetic moments adiabatically, i.e., it is always in its ground state with respect to the momentary configuration. Then it is possible to introduce (e.g., by the solution of the Kohn-Sham equations of the electronic density-functional theory for prescribed[11] directions $\mathbf{e_R}$) adiabatic single-electron energies $\varepsilon_i(\{\mathbf{e_R}(t)\})$, the

 

adiabatic Fermi-Dirac occupation numbers $f_i(\{\mathbf{e_R}(t)\})$, and an adiabatic Fermi surface $S(\{\mathbf{e_R}(t)\})$. When the orientational configuration changes in time, then this Fermi surface will be modified (breathing Fermi surface[4]). For a collinear magnetization, $\mathbf{e_R}(t)=\mathbf{e}(t)$, $S(\mathbf{e}(t))$ changes in time because the $\varepsilon_i$ depend on $\mathbf{e}(t)$ via the spin-orbit coupling. In a time-dependent noncollinear situation, the $\varepsilon_i$ change in addition because of the interatomic exchange interactions arising[12] in the density-functional theory from the dependence of the kinetic energy of the electronic system on $\{\mathbf{e_R}(t)\}$. Because these kinetic-energy interactions in general are much stronger than the spin-orbit interactions, stronger changes of the adiabatic Fermi surface can be expected for systems with time-dependent degree of noncollinearity. For the strictly adiabatic situation, quantum-mechanical arguments (see, e.g., Ref. 8, and references therein) yield the EOM

$$\frac{d\mathbf{e_R}}{dt} = -\frac{2\mu_B}{\hbar}\frac{1}{M_\mathbf{R}}\frac{\partial E}{\partial \mathbf{e_R}} \times \mathbf{e_R} = -\gamma \mathbf{e_R} \times \mathbf{H}_{\mathrm{eff},\mathbf{R}}, \tag{1}$$

with the total energy $E$ and $\gamma=-2\mu_B/\hbar$. This EOM looks like a Gilbert equation without the damping term, i.e., in the strictly adiabatic situation, there is no damping at all.

To introduce damping, we abandon the notion that the electronic systems is at any instant in its ground state with respect to the $\{\mathbf{e_R}(t)\}$. To do this for a situation close to the adiabatic limit, the breathing Fermi-surface model[4–8] uses a concept very similar to the one of the Drude theory of conductivity. The basic idea is to keep the adiabatic single-electron energies $\varepsilon_i(\{\mathbf{e_R}(t)\})$, but to replace the adiabatic occupation numbers $f_i(\{\mathbf{e_R}(t)\})$ by nonadiabatic occupation numbers $n_i(t)$. The reason is that a change of the Fermi surface $S(\{\mathbf{e_R}(t)\})$ requires electronic scattering processes and these scattering processes do not take place infinitely fast (as it has been assumed for the strictly adiabatic situation) but require finite time. This is accounted for by a relaxation-time ansatz,

$$\frac{dn_i(t)}{dt} = -\frac{1}{\tau_i}[n_i(t) - f_i(\{\mathbf{e_R}(t)\})]. \tag{2}$$

With the further approximation $\tau_i=\tau$ for all $i$, and for the case of a near-adiabatic situation where the characteristic time scale for the dynamics of the $\mathbf{e_R}(t)$ is much larger than $\tau$, the solution of Eq. (2) may be approximated by

$$n_i(t) = f_i(t) - \tau\frac{df_i(t)}{dt} + \ldots . \tag{3}$$

For the derivation of an EOM for the near-adiabatic time scale, we start from Eq. (1) and try to represent $\partial E/\partial \mathbf{e_R}$ by single-electron energies $\varepsilon_i(\{\mathbf{e_R}(t)\})$ and occupation numbers $f_i(\{\mathbf{e_R}(t)\})$ which we then can replace in the spirit of the breathing Fermi-surface model by the nonadiabatic occupation numbers $n_i(t)$ of Eq. (3). To achieve this we use a method closely related to the magnetic force theorem in the variant by Bruno,[13] which is an application of the Harris-Foulkes functional[14] to the magnetic system with the orientations of the atomic magnetic moments at sites $\mathbf{R}$ prescribed by Lagrangian fields $\mathbf{B}_\mathbf{R}^\lambda$.

We start by prescribing an initial orientational configuration $\{\mathbf{e}_\mathbf{R}^0\}$. The fields $\mathbf{B}_\mathbf{R}^{\lambda,0}$ which generate these directions of the moments are determined self-consistently[11] by a density-functional calculation. This calculation yields in addition the initial self-consistent spin-density matrix

$$\underline{\underline{\rho}}^0(\mathbf{r}) = n^0(\mathbf{r})\underline{\underline{1}} + m^0(\mathbf{r})\mathbf{e}_0^\mathbf{m}(\mathbf{r}) \cdot \underline{\underline{\boldsymbol{\sigma}}}. \tag{4}$$

Here $n^0(\mathbf{r})$ is the particle density, $\mathbf{m}^0(\mathbf{r})=m^0(\mathbf{r})\mathbf{e}_0^\mathbf{m}(\mathbf{r})$ denotes the continuous spin density with the continuous orientation field $\mathbf{e}_0^\mathbf{m}(\mathbf{r})$ (not to be mixed up with the $\mathbf{e}_\mathbf{R}^0$), $\underline{\underline{1}}$ is the unity matrix, and $\underline{\underline{\boldsymbol{\sigma}}}$ represents the vector of Pauli matrices. Furthermore, the calculation yields the effective potential matrix $\underline{\underline{W}}[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^{\lambda,0}]$, the single-electron eigenvalues $\varepsilon_i[\underline{\underline{W}}[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^{\lambda,0}]]$, the corresponding occupation numbers $f_i^0$, and the total energy $E[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^{\lambda,0}]$.

In a second step we prescribe a slightly different new orientational configuration,

$$\{\mathbf{e_R}\} = \{\mathbf{e}_\mathbf{R}^0 + \delta\mathbf{e_R}\} = \{\mathbf{R_R} \cdot \mathbf{e}_\mathbf{R}^0\}, \tag{5}$$

with the local rotations $\mathbf{R_R} \in \mathrm{SO}(3)$ at sites $\mathbf{R}$. In a second density-functional calculation we then determine again in a self-consistent manner the Lagrangian fields $\mathbf{B}_\mathbf{R}^\lambda$ which are required to generate the new directions $\{\mathbf{e_R}\}$. The only scope of this second self-consistent calculation is the determination of the numerically exact fields $\mathbf{B}_\mathbf{R}^\lambda$. We do not make use of the self-consistently determined energy $E[\underline{\underline{\rho}};\mathbf{B}_\mathbf{R}^\lambda]$ which would enable us to calculate numerically the difference $\delta E = E[\underline{\underline{\rho}};\mathbf{B}_\mathbf{R}^\lambda] - E[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^{\lambda,0}]$ but would not allow us to introduce the breathing Fermi-surface model.[15] For the following, we consider the Lagrangian fields $\mathbf{B}_\mathbf{R}^{\lambda,0}$ and $\mathbf{B}_\mathbf{R}^\lambda$ as external fields $\mathbf{B}_\mathbf{R}^0$ and $\mathbf{B_R}$, and we calculate the energy difference between the two configurations by the extended Harris-Foulkes approach described by Bruno (Ref. 13).

To do this, we construct an input spin-density matrix

$$\underline{\underline{\rho}}^{\mathrm{in}}(\mathbf{r}) = n^0(\mathbf{r})\underline{\underline{1}} + m^0(\mathbf{r})[\mathbf{R_R} \cdot \mathbf{e}_0^\mathbf{m}(\mathbf{r})] \cdot \underline{\underline{\boldsymbol{\sigma}}}, \tag{6}$$

i.e., we rotate the initial spin density within the atomic spheres at sites $\mathbf{R}$ by the rotation matrix $\mathbf{R_R}$ defined above. We then solve the Kohn-Sham equation for the fixed potential matrix $\underline{\underline{W}}[\underline{\underline{\rho}}^{\mathrm{in}};\mathbf{B_R}]$ constructed from $\underline{\underline{\rho}}^{\mathrm{in}}$ and $\mathbf{B_R}$, yielding the single electron energies $\varepsilon_i^{\mathrm{HF}}[\underline{\underline{W}}[\underline{\underline{\rho}}^{\mathrm{in}};\mathbf{B_R}]]$ and the corresponding occupation numbers $f_i^{\mathrm{HF}}=f(\varepsilon_i^{\mathrm{HF}})$. Following the arguments of Bruno,[13] the energy difference $\delta E$ then is calculated by use of the Harris-Foulkes functional[14] $E^{\mathrm{HF}}$ generalized to noncollinear magnetic systems,[13] yielding

$$\begin{aligned}\delta E &= E^{\mathrm{HF}}[\underline{\underline{\rho}}^{\mathrm{in}};\mathbf{B_R}] - E[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^0] + \mathcal{O}_2(\delta n^{\mathrm{in}}, \delta\mathbf{m}^{\mathrm{in}}) \\ &= \sum_i f(\varepsilon_i^{\mathrm{HF}})\varepsilon_i^{\mathrm{HF}}[\underline{\underline{W}}[\underline{\underline{\rho}}^{\mathrm{in}};\mathbf{B_R}]] - \sum_i f(\varepsilon_i)\varepsilon_i[\underline{\underline{W}}[\underline{\underline{\rho}}^0;\mathbf{B}_\mathbf{R}^0]] \\ &\quad + \mathcal{O}_2(\delta n^{\mathrm{in}}, \delta\mathbf{m}^{\mathrm{in}}).\end{aligned} \tag{7}$$

In Eq. (7), $\delta X^{\mathrm{in}}$ with $X=n,\mathbf{m}$ are the differences between the input quantities according to Eq. (6) and the corresponding quantities which would be obtained by a self-consistent calculation for the $\{\mathbf{B_R}\}$.

The $f(\varepsilon_i^{\mathrm{HF}})$ and $\varepsilon_i^{\mathrm{HF}}$ depend on the configuration (5). Performing a Taylor expansion of these quantities, neglecting

terms of $\mathcal{O}_2(\delta\mathbf{e}_\mathbf{R})$, and taking into account $\varepsilon_i^{\mathrm{HF}}(\{\mathbf{e}_\mathbf{R}^0\}) = \varepsilon_i(\{\mathbf{e}_\mathbf{R}^0\})$ yields

$$\delta E = \sum_i f_i \left.\frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_\mathbf{R}}\right|_{\mathbf{e}_\mathbf{R}^0} \cdot \delta\mathbf{e}_\mathbf{R} + \sum_i \left.\frac{\partial f_i}{\partial \mathbf{e}_\mathbf{R}}\right|_{\mathbf{e}_\mathbf{R}^0} \cdot \varepsilon_i(\{\mathbf{e}_\mathbf{R}^0\})\delta\mathbf{e}_\mathbf{R}. \quad (8)$$

Assuming that changes of the $f_i$ due to orientational changes occur only for states close to the Fermi level $\varepsilon_\mathrm{F}$ yields for the last term of Eq. (8)

$$\varepsilon_F \sum_i \delta f_i = 0, \quad (9)$$

where we have used in Eq. (9) that the total number of states is conserved. With $\partial E/\partial \mathbf{e}_\mathbf{R} = \partial \delta E/\partial \delta \mathbf{e}_\mathbf{R}$, we then obtain

$$\frac{\partial E}{\partial \mathbf{e}_\mathbf{R}} = \sum_i f_i \left.\frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_\mathbf{R}}\right|_{\mathbf{e}_\mathbf{R}^0}, \quad (10)$$

where the derivative can be calculated numerically from [with $\varepsilon_i^{\mathrm{HF}}(\{\mathbf{e}_\mathbf{R}^0\}) = \varepsilon_i(\{\mathbf{e}_\mathbf{R}^0\})$]

$$\left.\frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_\mathbf{R}}\right|_{\mathbf{e}_\mathbf{R}^0} = \lim_{\delta\mathbf{e}_\mathbf{R}\to 0} \frac{\varepsilon_i^{\mathrm{HF}}(\{\mathbf{e}_\mathbf{R}^0 + \delta\mathbf{e}_\mathbf{R}\}) - \varepsilon_i(\{\mathbf{e}_\mathbf{R}^0\})}{\delta\mathbf{e}_\mathbf{R}}. \quad (11)$$

Following the general approach of the breathing Fermi-surface model, the EOM for the near-adiabatic situation can be obtained by inserting Eq. (10) into Eq. (1) and replacing the adiabatic occupation numbers $f_i$ by the nonadiabatic occupation numbers $n_i$ of Eq. (3). Finally, the chain rule is used,

$$\frac{df_i}{dt} = \frac{\partial f_i}{\partial \varepsilon_i} \sum_\mathbf{R} \frac{\partial \varepsilon_i}{\partial \mathbf{e}_\mathbf{R}} \frac{d\mathbf{e}_\mathbf{R}}{dt}, \quad (12)$$

yielding the fundamental result

$$\frac{d\mathbf{e}_\mathbf{R}}{dt} = -\gamma \mathbf{e}_\mathbf{R} \times \mathbf{H}_{\mathrm{eff},\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}''}\}) + \mathbf{e}_\mathbf{R} \times \sum_{\mathbf{R}'} \mathbf{A}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\}) \cdot \frac{d\mathbf{e}_{\mathbf{R}'}}{dt}, \quad (13)$$

$$\mathbf{H}_{\mathrm{eff},\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}''}\}) = \frac{1}{M_\mathbf{R}} \sum_i f_i \frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_\mathbf{R}}, \quad (14)$$

$$\frac{1}{\tau}\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\}) \cdot \frac{d\mathbf{e}_{\mathbf{R}'}}{dt} = -\frac{\gamma}{M_\mathbf{R}} \sum_i \frac{\partial f_i}{\partial \varepsilon_i} \frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_\mathbf{R}} \frac{\partial \varepsilon_i^{\mathrm{HF}}}{\partial \mathbf{e}_{\mathbf{R}'}} \cdot \frac{d\mathbf{e}_{\mathbf{R}'}}{dt}. \quad (15)$$

It should be noted that the second term of Eq. (13) can be decomposed into a relaxation torque and a term modifying the precession.[6] Equation (13) has the general appearance of a Gilbert[16] equation, with a term describing the precession in an effective field $\mathbf{H}_{\mathrm{eff},\mathbf{R}}$ and a damping term, however, with the damping constant $\alpha$ appearing in the Gilbert equation being replaced by damping matrices $\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\})$ which depend on the orientational configuration $\{\mathbf{e}_{\mathbf{R}''}\}$ of the whole system because the $\partial \varepsilon_i^{\mathrm{HF}}/\partial \mathbf{e}_\mathbf{R}$ depend on the configuration. For a collinear situation, this means an anisotropic damping, i.e., $\mathbf{A}$ depends on the orientation of the magnetization in the system, as has been shown explicitly numerically[5,6,8] (with a slightly different calculational method) for bulk Fe, Co, and Ni. For monatomic layers and wires of these materials, there are even orientations for which the damping vanishes.[6,8] For a noncollinear situation it means that the damping is in addition nonlocal. This is certainly relevant for strongly noncollinear systems like narrow domain walls[17] or vortices,[1] where we expect stronger damping than for collinear situations because the $\partial \varepsilon_i^{\mathrm{HF}}/\partial \mathbf{e}_\mathbf{R}$ are larger (see above). It is well known for a long time that the effective field $\mathbf{H}_{\mathrm{eff},\mathbf{R}}$ (which also contains the $\partial \varepsilon_i^{\mathrm{HF}}/\partial \mathbf{e}_\mathbf{R}$) is both anisotropic (described in a micromagnetic theory by the magnetocrystalline anisotropy energy) and nonlocal (described by the micromagnetic exchange energy), whereas for the damping these two features have often been overlooked so far.

As a confirmation of the expectation of stronger damping in noncollinear systems, we calculate the matrix $\mathbf{A}/\tau$ for a noncollinear configuration in hcp Co. The directions $\{\mathbf{e}_\mathbf{R}\}$ of the two atomic magnetic moments in the unit cell enclose an angle of 2° or of 5°. Typical angles between nearest-neighbor moments in domain walls of uniaxial materials are 2° for a 180° Bloch wall in Co or 3° (5°) for a 180° Néel wall in Co ($Pr_2Fe_{14}B$). The derivatives (11) are only determined by interatomic exchange because spin-orbit coupling was switched off in this calculation. For symmetry reasons only one eigenvalue $\tilde{\alpha}$ of $\mathbf{A}$ is nonzero. We get $\tilde{\alpha}\mu_B^2 M_\mathbf{R}/\hbar^2\gamma\tau \approx 11 \cdot 10^{20}$ s$^{-2}$ ($65 \cdot 10^{20}$ s$^{-2}$) for an angle of 2° (5°), where the value for 5° is about one order of magnitude larger than the value obtained for a collinear configuration in this system with spin-orbit coupling.[6,8]

Equation (15) shows that the damping is proportional to $\tau$ and hence to the conductivity. Experimentally[18] this proportionality has been found for single crystals of Ni at low temperatures $T$, whereas at high $T$ a proportionality of $\alpha$ to the resistivity $\rho = 1/\sigma \sim \tau$ has been observed. According to Refs. 8 and 19, it is expected that the contribution $\mathbf{A} \sim \sigma$ arises from intraband transitions for which the breathing Fermi-surface model holds and which dominate at low $T$ whereas the contribution $\mathbf{A} \sim \rho$ is related to interband transitions which are not accounted for by the model. (For a theory of the temperature dependence of damping, see Ref. 19.) Accordingly, there are strong hints[20] that for Ni at low $T$ the damping is anisotropic (whereas for Fe and Co no observations in this direction have been reported so far). All the considerations of the paragraph are for collinear situations. Because in our theory, the damping matrix is proportional to $\tau$ both for collinear and noncollinear situations, we assume that in both situations, the theory is valid only as long as intraband transitions dominate, i.e., at low $T$.

To conclude, we managed to unify the breathing Fermi-surface model of magnetization damping for collinear as well as for noncollinear magnetization configurations. It appears that in this model the damping is both anisotropic and nonlocal, in contrast to the isotropic and local Gilbert damping.

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